2020

ARO YEAR IN REVIEW

U.S. Army Combat Capabilities Development Command (DEVCOM)
Army Research Laboratory (ARL) • Army Research Office (ARO)
P.O. Box 12211 • Research Triangle Park, NC 27709-2211

ARO Year in Review 2020

This document provides the annual historical record of the Army Research Office (ARO) programs for fiscal year 2020 (FY20), including program goals, management strategies, funding information, and key accomplishments.

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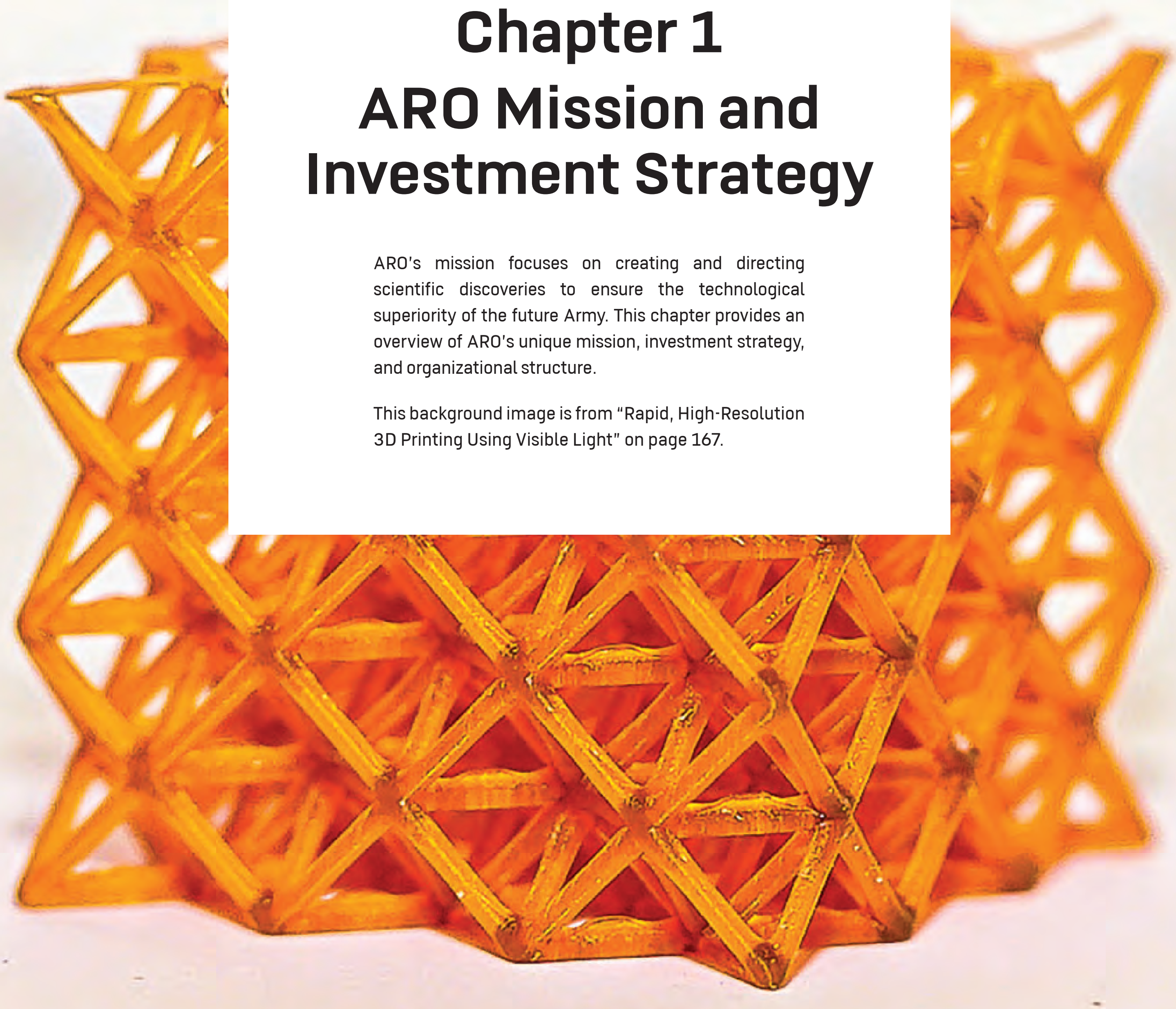
Chapter 1
ARO Mission and Investment Strategy

ARO's mission focuses on creating and directing scientific discoveries to ensure the technological superiority of the future Army. This chapter provides an overview of ARO's unique mission, investment strategy, and organizational structure.

This background image is from "Rapid, High-Resolution 3D Printing Using Visible Light" on page 167.



Message from the Director

The Army Research Office (ARO) is dedicated to extending the frontiers of science for the benefit of the Soldier. As the extramural basic research funding arm of the U.S. Army Combat Capabilities Development Command Army Research Laboratory, ARO is the Army's agency for linking the power of the global academic research community with the future of national defense.

In ARO Year in Review, our annual report for fiscal year 2020, we share with you the science we discovered that could change the world.

In addition to presenting our annual financial performance and investment strategy, ARO Year in Review showcases ARO's support of national and international transformational extramural basic science research.

For 70 years, ARO has served as the Army's principal agent for the planning, organization, selection, and management of extramural basic research in response to Army-wide requirements. Magnified by 2020's extraordinary challenges, scientists we funded pivoted, discovered, achieved, and built upon this legacy of innovation in the physical, engineering, and information sciences. From accelerating research at the forefront of quantum computing to leveraging our relationships with academia and industry to discover potential countermeasures against COVID-19, the research efforts supported by ARO continue to fuel innovation and address requirements that will enable crucial future Army technologies and capabilities.

ARO strives to embrace inclusivity by providing opportunities for research and education to students from all sectors of our society. From high school through advanced degrees, we coordinate programs designed to foster and engage talent within science, technology, engineering, and mathematics (STEM) disciplines. Additionally, we honor our commitment to equality of opportunity through support of socio-economically disadvantaged and diverse academic institutions. The Nation must be prepared for a world increasingly dependent on STEM capabilities, and investment in our youth ensures the United States maintains its technological superiority.

ARO's commitment to sustaining cutting-edge research is made possible by aligning with rigorous internal and external review and evaluation methods, such as the National Academies of Sciences Technical Assessment Board (TAB). By successfully demonstrating the highest standards of research and discovery in its core funding landscape, we continue to create and leverage opportunities to collaborate with other DoD stakeholders in the tireless pursuit of technological and scientific advancement.

It is ARO's commitment toward active program management and understanding in the nonlinearity of science that allows us to identify high-risk, high-payoff investments in science and engineering research and education. The bold and far-reaching projects of the past year continue to illustrate ARO's unique ability to create synergies between basic research and transformational impact, ultimately supporting the Army's quest to forge the future.

Dr. Barton H. Halpern

Director, Army Research Office
DEVCOM Army Research Laboratory

Who We Are and What We Do

The Army Research Office (ARO) is part of the U.S. Army Futures Command (AFC) – U.S. Army Combat Capabilities Development Command (DEVCOM, formerly CCDC) – Army Research Laboratory (ARL), the Army's corporate research laboratory. Founded in 1951 and based in Research Triangle Park, North Carolina, ARO comprises more than 100 scientists, engineers, and support staff who manage the Army's extramural research program to create new and innovative scientific discoveries that will enable crucial capabilities and ensure technological superiority of the future Army.

ARO Mission

The mission of ARO is to create and direct scientific discoveries for revolutionary new Army capabilities, drive science to develop solutions to existing Army technology needs, accelerate the transition of basic research, educate and train the future Army Scientists and Engineers (S&E) workforce, create technological superiority for U.S. Forces, and prevent adversary technological surprise.

ARO serves as the Army's principal agent for the planning, organization, selection, and management of extramural basic research in response to Army-wide requirements in the following scientific disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. ARO utilizes the vast intellectual capital of the world's research organizations to accomplish the following:

- Drive science to develop unprecedented Army capabilities and solutions to existing Army technology needs.
- Conceive of and exploit scientific opportunities for knowledge products.
- Leverage science and technology (S&T) to both create and prevent technological overmatch.
- Create and strengthen the partnerships among academia, industry, and government.
- Educate and train the future science and engineering workforce for the Army and DoD.
- Accelerate the transition of basic science research.

DID YOU KNOW?

Basic research is defined by the DoD as "systematic study directed toward greater knowledge or understanding of the fundamental aspects of phenomena and of observable facts without specific applications towards processes or products in mind" (DoD 7000.14-R Volume 2B, Chapter 5, 2017).

ARO aims to generate new scientific discoveries and innovative advances by funding high-risk, high-payoff research opportunities, principally at universities, but also with large and small businesses. These efforts support and drive the realization of the Army Functional Concepts, and the ARL Competencies and Essential Research Programs (ERPs). The results of these efforts are transitioned to the Army research and development community, industry, or academia to ensure technological superiority of our Soldiers, Army, and Nation.

ARO Investment Strategy

ARO executes its mission through a long-range investment strategy designed to generate cutting-edge scientific discoveries that address the expanding range of present and future operational challenges, ultimately ensuring land force overmatch. The ARO research portfolio consists principally of extramural academic research efforts including single investigator efforts, university affiliated research centers, and specially tailored outreach programs. ARO program managers competitively select and fund basic research proposals from educational institutions, nonprofit organizations, and private industry. Each program has its own objectives and set of advantages as described further in Chapter 2.

ARO's mission represents the most long-range Army view for new scientific discovery to initiate disruptive new technology, with system applications often 20-30 years away.

ARO's investment strategy represents the most long-range Army view for new scientific discovery to initiate disruptive new technology, with system applications often 20-30 years away. This investment directly supports the ARL-wide research strategy, which is organized into 11 Competencies. Current areas of emphasis are also designated by ARL's ERPs, which aim to address particular technology gaps for the current and future Army. Additionally, ARO programs and research areas are aligned with the research priorities set within the DoD: the Army Modernization Priorities, the Army Functional Concepts, and the Assistant Secretary of Defense for Research and Engineering S&T Priorities.

While the ARL Directorates are the primary users of the results generated through ARO's research programs, ARO also supports research of interest for all the DEVCOM Centers, the U.S. Army Corps of Engineers (USACE), the U.S. Army Medical Research and Development Command (USAMRMC), and other Army Commands and DoD agencies. The coordination of the ARO extramural research program and joint proposal monitoring with ARL Directorates, DEVCOM Centers, and other Army organizations ensures a highly productive and cost-effective Army research effort.

Coordination for Program Development and Monitoring

To ensure complementary investment strategies, ARO's extramural research programs are formulated in concert with the DEVCOM Centers and ARL-wide strategy (in addition to other Army Commands and DoD agencies). This coordination includes, but is not limited to, the following:

DEVCOM CENTERS

Armaments Center (DEVCOM AC)

Army Research Laboratory (DEVCOM ARL)

Aviation and Missile Center (DEVCOM AvMC)

Chemical Biological Center (DEVCOM CBC)

Command, Control, Computers, Communications, Cyber, Intelligence, Surveillance and Reconnaissance Center (DEVCOM C5ISR)

Data & Analysis Center (DEVCOM DAC)

Ground Vehicle Systems Center (DEVCOM GVSC)

Soldier Center (DEVCOM SC)

ARL DIRECTORATES

Computational and Information Sciences Directorate (ARL CISD)

Human Research and Engineering Directorate (ARL HRED)

Sensors and Electron Devices Directorate (ARL SEDD)

Weapons and Materials Research Directorate (ARL WMRD)

ARL COMPETENCIES

Sciences of Extreme Materials

This Competency investigates the "mechanical" response, related manufacturing methods, and performance extremes of materials, including active, adaptive, and flexible/soft materials, as well as novel manufacturing for energetic materials.

Humans in Complex Systems

This Competency leverages multidisciplinary, non-medical approaches to understand and modify the potential of humans situated in and interacting within complex social, technological, and socio-technical systems.

Electromagnetic Spectrum Sciences

This Competency aims to develop novel approaches to sensing, counter-sensing, and protection of sensing as well as testing emerging concepts for lasers, direct-energy weapons, propagation, radio frequency devices, radars, and electronic warfare.

Photonics, Electronics, and Quantum Sciences

This Competency studies the materials, manufacturing methods, and devices required for achieving photonic, electronic, and quantum-based effects.

Network Science and Computational Sciences

This Competency seeks science that enables and ensures secure resilient communication networks to facilitate distributed analytics in multi-domain operations (MDO).

Energy Sciences

This Competency concentrates on the science of mechanical and electrical power generation storage, conditioning, and distribution, as well as energy conversion.

Military Information Sciences

This Competency focuses on discovering the underpinning sciences and enablers required to provide timely, mission-aware information to humans and systems at speed and scale to support all-domain and coalition operations.

Terminal Effects

This Competency invests in research dedicated to better understanding weapon-target interactions.

Mechanical Sciences

This Competency investigates the science of physical robotics and autonomy, novel mechanics, mechanisms, and control, leveraging innovations in artificial intelligence and unmanned ground and air vehicle concepts.

Biological and Biotechnology Sciences

This Competency explores innovative biologically related research topics, including synthetic biology, incapacitation and degradation, and augmentation.

Weapons Sciences

This Competency examines the science of internal, transitional, and external ballistics as well as the launch, flight, control, and navigation of guided weapons.

ARL ESSENTIAL RESEARCH PROGRAMS (ERPs)

Artificial Intelligence for Maneuver and Mobility (AIMM)

Emerging Overmatch Technologies (EOT)

Foundational Research for Electronic Warfare in Multi-Domain Operations (FREEDOM)

Human Autonomy Teaming (HAT)

Long-Range Distributed and Cooperative Engagements (LRDCE)

Physics of Soldier Protection for Defeat of Evolving Threats (PSP)

Quantum-Precision Navigation and Timing (QIS-PNT)

Science of Additive Manufacturing for Next Generation Munitions (SAMM)

Transformational Synthetic Biology for Military Environments (TRANSFORME)

Versatile Tactical Power and Propulsion (VICTOR)

ARO Organizational Structure

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific Branches are aligned to a specific scientific discipline (e.g., physics), with outreach activities managed through the Technology Integration and Outreach Branch, and organization-wide support provided by the Operations and Financial Management Offices (Figure 1).

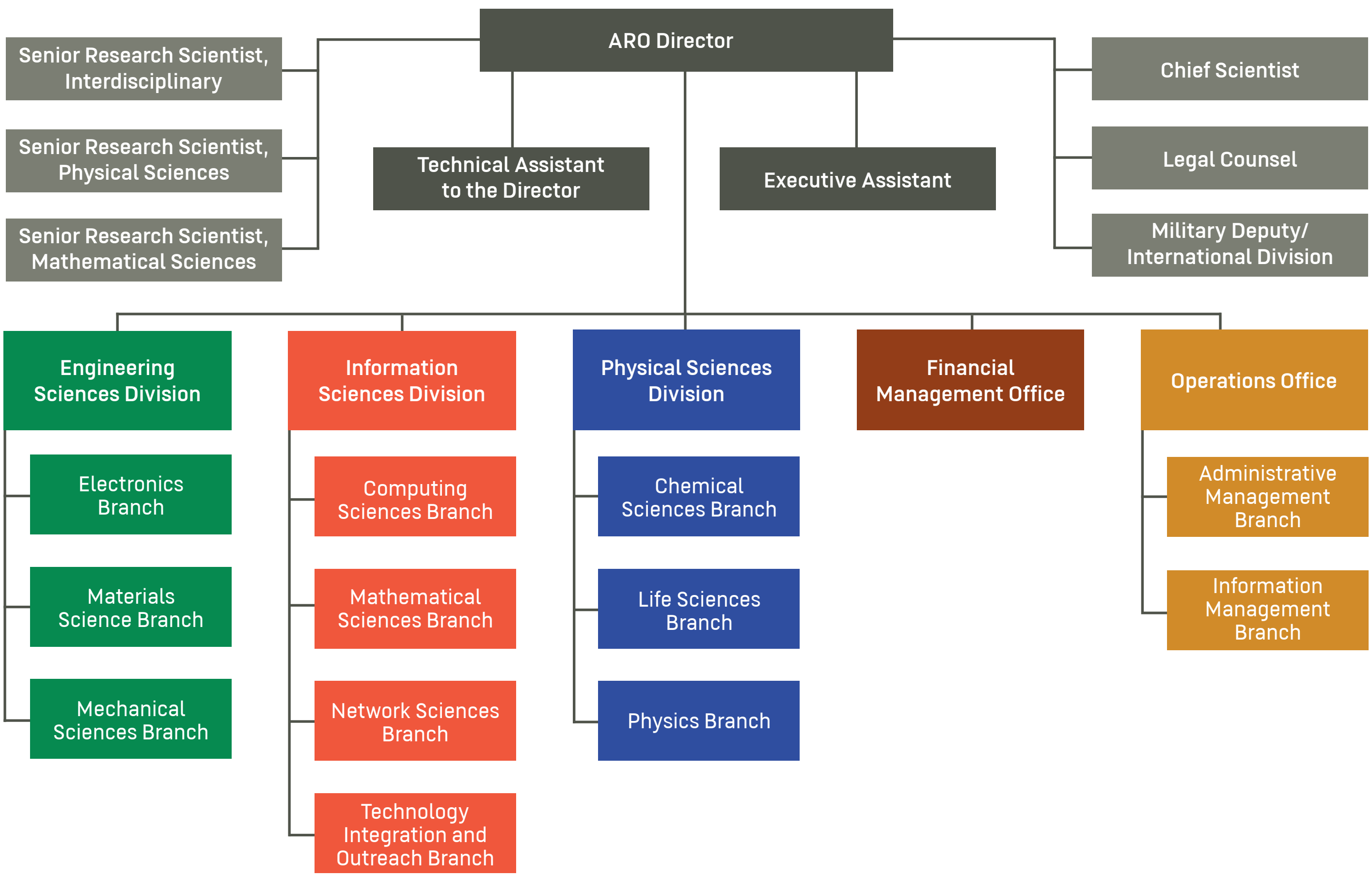


Figure 1: ARO's scientific Branches fall under the Physical Sciences, Engineering Sciences, and Information Sciences Divisions.

ARO Staff

DIRECTOR'S OFFICE

Dr. Barton H. Halpern
Director

Mr. John Stone, Esq.
Legal Counsel

Ms. Tisha Torgerson
Executive Assistant

Dr. Matthew Munson
Technical Assistant to the Director (Acting)

CHIEF SCIENTIST

Dr. David Stepp

SENIOR RESEARCH SCIENTISTS

Dr. Stephen Lee
Interdisciplinary Sciences

Dr. Peter Reynolds
Physical Sciences

Dr. Bruce West
Mathematical Sciences

INTERNATIONAL DIVISION

LTC David Dykema
Military Deputy, Division Chief

Dr. Wesley Henderson
Program Manager, ***Energy Transport and Storage***

Dr. Frederick Gregory
Program Manager, ***Human Dimension***

Dr. Robert Ulman
Program Manager, ***Network Science and Intelligent Systems***

Dr. Thomas Bahder
Program Manager, ***Quantum Scale Materials***

Dr. Valerie Martindale
Program Manager, ***Synthetic Biology***

ENGINEERING SCIENCES DIVISION (ESD)

Dr. Chakrapani (Pani) Varanasi
Division Chief (Acting)

Dr. Larry Russell
Program Manager, ***University Research Initiative***

Mr. Anthony Wong
General Engineer

Ms. Liza Wilder
Administrative Specialist

ELECTRONICS BRANCH

Dr. Marc Ulrich
Branch Chief (Acting)

Dr. Albena Ivanisevic
Program Manager, ***Biotronics***

Dr. Tania Paskova
Program Manager, ***Electronic Sensing***

Dr. Michael Gerhold
Program Manager, ***Optoelectronics***

Dr. Joe Qiu
Program Manager, ***Solid-State Electronics and Electromagnetics***

MATERIALS SCIENCE BRANCH

Dr. Dawanne Poree
Branch Chief (Acting)

Dr. Evan Runnerstrom
Program Manager, ***Materials Design***

Dr. Chakrapani (Pani) Varanasi
Program Manager, ***Physical Properties of Materials***

Dr. Daniel Cole
Program Manager, ***Mechanical Behavior of Materials***

Dr. Michael Bakas
Program Manager, ***Synthesis and Processing of Materials***

MECHANICAL SCIENCES BRANCH

Dr. Ralph Anthenien
Branch Chief, Program Manager, ***Propulsion and Energetics***

Dr. Samuel Stanton
Program Manager, ***Complex Dynamics and Systems***

Dr. Julia Barzyk
Program Manager, ***Earth Materials and Processes***

Dr. Matthew Munson
Program Manager, ***Fluid Dynamics***

Dr. Denise Ford
Program Manager, ***Solid Mechanics***

INFORMATION SCIENCES DIVISION (ISD)

Dr. Randy Zachery
Division Chief

Mr. Tylar Temple
General Engineer

Ms. Debra Brown
Administrative Specialist

Ms. Diana Pescod
Administrative Support Assistant

COMPUTING SCIENCES BRANCH

Dr. Purush Iyer
Branch Chief, Program Manager, *Knowledge Systems, University Affiliated Research Centers (UARCs)*

Dr. J. Michael Coyle
Program Manager, *Computational Architecture and Visualization*

Dr. MaryAnne Fields
Program Manager, *Cyber Intelligent Systems*

Dr. Hamid Krim
Program Manager, *Information Processing and Fusion*

MATHEMATICAL SCIENCES BRANCH

Dr. Joseph Myers
Branch Chief, Program Manager, *Computational Mathematics*

Dr. Virginia Pasour
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Dr. Radhakrishnan Balu
Program Manager (Acting), *Modeling of Complex Systems*

Dr. Michael Lavine
Program Manager, *Probability and Statistics*

NETWORK SCIENCES BRANCH

Dr. Cliff Wang
Branch Chief, Program Manager, *Information Assurance*

Dr. Derya Cansever
Program Manager, *Multi-Agent Network Control*

Dr. Edward Palazzolo
Program Manager, *Social and Cognitive Networks*

Dr. Robert Ulman
Program Manager, *Wireless and Hybrid Communications Networks*

TECHNOLOGY INTEGRATION AND OUTREACH BRANCH

Mr. Michael Caccuitto
Branch Chief, Program Manager (Acting), *Department of the Army Small Business Technology Transfer (STTR) Program*

Ms. Nicole Fox
Program Manager, ARO Small Business *Innovation Research (SBIR) and STTR Programs*

Ms. Patricia Huff
Program Manager, *Historically Black Colleges and Universities/Minority-Serving Institutions (HBCUs/MIs) Program*

Ms. Jennifer Ardouin
Program Manager, *Education Outreach*

PHYSICAL SCIENCES DIVISION (PSD)

Dr. Hugh De Long
Division Chief

Dr. Kelby Kizer
General Physical Scientist

Dr. James Burgess
Program Manager, *UARCs*

Mr. John McConville
Technology Transfer Officer, *UARCs*

Ms. Ivory Chaney
Administrative Specialist

CHEMICAL SCIENCES BRANCH

Dr. Robert Mantz
Branch Chief, Program Manager, *Electrochemistry*

Dr. Elizabeth King-Doonan
Program Manager, *Environmental Chemistry*

Dr. James Parker
Program Manager, *Molecular Structure and Dynamics*

Dr. Dawanne Poree
Program Manager, *Polymer Chemistry,* Program Manager (Acting), *Reactive Chemical Systems*

LIFE SCIENCES BRANCH

Dr. Micheline (Mimi) Strand
Branch Chief, Program Manager, *Genetics*

Dr. Stephanie McElhinny
Program Manager, *Biochemistry*

Dr. Robert Kokoska
Program Manager, *Microbiology*

Dr. Frederick Gregory
Program Manager, *Neurophysiology of Cognition*

Dr. Lisa Troyer
Program Manager, *Social and Behavioral Sciences*

PHYSICS BRANCH

Dr. Edward Palazzolo
Branch Chief (Acting)

Dr. Marc Ulrich
Program Manager, *Solid State Physics*

Dr. Paul Baker
Program Manager, *Atomic and Molecular Physics*

Dr. T. R. Govindan
Program Manager (NASA), *Quantum Computation and Networking*

Dr. Sara Gamble
Program Manager, *Quantum Information Science (QIS)*

Dr. James Joseph
Program Manager, *Quantum Optics*

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Mr. Richard Black
Management Analyst

Ms. Janelle Cato
Management Analyst

Ms. Carla Changer
Accountant

Ms. Sandra Elizondo
Accountant

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Associate Director

Ms. Christine Doss
Administrative Officer

Ms. Wanda Wilson
Administrative Officer

ADMINISTRATIVE MANAGEMENT BRANCH

Mr. Rich Freed
Branch Chief

Ms. Peggy Lee
Management Analyst

Mr. Scott Petty
Security Manager

Mr. Klinton Snead
Operations Officer

INFORMATION MANAGEMENT BRANCH

Mr. Jack Rappold
Branch Chief

Mr. Russell Errett
Computer Engineer

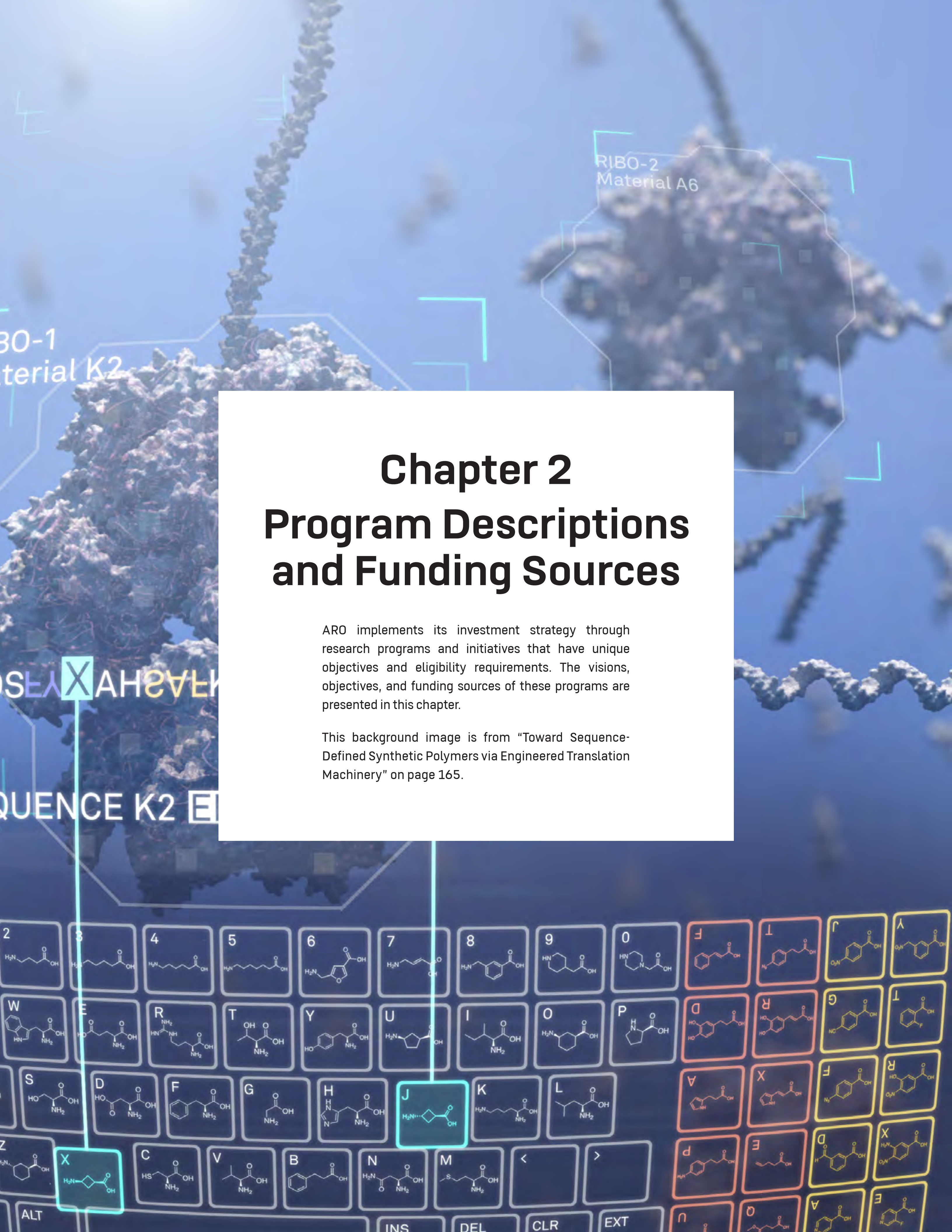
Mr. Krishna Sambangi
Computer Scientist

Mr. James Ward
Computer Scientist

Mr. Jimmy Bass
IT Specialist

Mr. Barry Pulliam
Network Engineer

Ms. Carla Davis
Program Specialist



Chapter 2
Program Descriptions and Funding Sources

ARO implements its investment strategy through research programs and initiatives that have unique objectives and eligibility requirements. The visions, objectives, and funding sources of these programs are presented in this chapter.

This background image is from "Toward Sequence-Defined Synthetic Polymers via Engineered Translation Machinery" on page 165.

Program Descriptions and Funding Sources

ARO pursues a variety of investment strategies to meet its mission to create and direct scientific discoveries for revolutionary new Army capabilities. ARO, as part of DEVCOM ARL, is a critical provider of fundamental discoveries in support of all ARL Competencies and Essential Research Programs (ERPs). ARO implements its investment strategy through research programs and initiatives that have unique objectives and eligibility requirements. The visions, objectives, and funding sources of these programs are presented in this chapter.

The selection of proposal topics, proposal evaluation, and project monitoring are organized within ARO Branches according to scientific discipline (refer to Chapter 1, Figure 1). Each Branch devises a research strategy and develops topics to be included in the ARO Core Broad Agency Announcement (BAA; see Appendix [online only]). Researchers are encouraged to submit white papers and proposals in areas that support a Branch's objectives. The ARO Branches are not confined to only funding research in the academic departments that align with the Branch names; they have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea. Further, research topics that may align with more than one ARO program may be co-managed across Branches and Divisions in order to advance the interdisciplinary basic research needs of the broader scientific community.

Overview of Program Funding Sources

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant and contract monitoring of programs funded through a variety of DoD agencies, as described in the following subsections.

Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO. These include the following:

- The ARO Core Research Program, funded through the Army's basic research funds
- Three University Affiliated Research Centers (UARCs)
- The University Research Initiative (URI), which is overseen by the Office of the Secretary of Defense (OSD), and is divided into three component programs:
  - Multidisciplinary University Research Initiative (MURI)
  - Presidential Early Career Award for Scientists and Engineers (PECASE)
  - Defense University Research Instrumentation Program (DURIP)

ARO also participates in the Army-wide Small Business Innovation Research (SBIR) Program and manages the Small Business Technology Transfer (STTR) Program. In contrast to the basic research programs managed by ARO, the SBIR and STTR Programs focus primarily on feasibility studies leading to prototype demonstration of technology for specific applications.

OSD Funding

The programs managed or supported by ARO that are funded by OSD include the following:

- The Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCUs/MIs)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships
- High School Apprenticeship and Undergraduate Research Apprenticeship Programs

These activities are mandated by the DoD's Chief Technology Office, the Office of the Under Secretary of Defense for Research and Engineering [OUSD(R&E)]. ARO has been designated by OUSD(R&E) as the lead agency for the implementation of REP for HBCUs/MIs activities on behalf of the Tri-Service research offices—ARO, the Air Force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR).

External Funding Sources

In addition to the Army and OSD funds that directly support ARO's mission, ARO is in the unique position to also leverage funds from other stakeholders. These funds come from a variety of sources including other Army (e.g., U.S. Army Corps of Engineers [USACE], U.S. Army Medical Research and Development Command [USAMRDC], and U.S. Special Operations Command [SOCOM]) and broader DoD (e.g., ONR, AFOSR, Defense Advanced Research Project Agency [DARPA], and Defense Threat Reduction Agency [DTRA]) organizations. While the investment strategy for leveraged funds is comparable to the investment strategy for other ARO programs, these funds often support programs with basic research needs identified by the stakeholder. As such, the external funding landscape is fluid and can change on an annual basis depending on the specific research needs of the stakeholder and technology transition opportunities made possible by ARO Program Managers (PMs).

Overview of Program Descriptions

ARO Core Research Program

The ARO Core Research Program represents the primary or "core" mechanism ARO uses to solicit and execute long-term basic research that will lead to critical new or enhanced capabilities for the future Army. Within the ARO Core Research Program, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in the physical, engineering, and information sciences.

SINGLE INVESTIGATOR (SI) PROGRAM

The goal of the SI Program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously open, worldwide BAA solicitation. The grant awards in the SI Program typically support one or more faculty members plus graduate students and/or postdoctoral researchers for up to three years. The short grant cycle allows approximately one third of the extramural portfolio to be reinvested into new or advancing areas each year, which provides the Army with a dynamic method for rapidly investing or divesting in research.

EARLY CAREER PROGRAM (ECP)

The objective of the ECP, formerly the Young Investigator Program (YIP), is to attract outstanding, early career university faculty to Army-relevant research questions, to support their research, and encourage their teaching and research careers. Exceptional ECP projects may be considered for the prestigious PECASE.

SHORT-TERM INNOVATIVE RESEARCH (STIR) PROGRAM

The objective of the STIR Program is to explore high-risk, proof-of-concept ideas within a nine-month time frame. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort produces promising results, the investigator may be encouraged to submit a proposal for longer-term funding options, such as an SI Program award.

CONFERENCES, WORKSHOPS, AND SYMPOSIA SUPPORT (CF) PROGRAM

The CF Program provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. Through this program, ARO supports and conducts scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation.

RESEARCH INSTRUMENTATION (RI) PROGRAM

The RI Program is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense by providing funds to purchase instrumentation in support of new research capabilities. The RI Program represents a small percentage of the total funds ARO invests in new research capabilities, with the majority of instrumentation support awarded through the DURIP.

INTERNATIONAL PROGRAM

The International Program is part of ARO's comprehensive approach to ensure that Army basic research funds are used to support the scientists who are best suited to drive high-risk, high-payoff Army relevant research. The research areas that make up the International Program were identified as areas where the forerunners of the field were located in institutions outside the U.S., and thus had fewer collaborative opportunities with existing Army and DoD programs. In FY20, ARO placed the management of the International Program under the MILDEP for unity of command. The MILDEP collaborated with the DEVCOM Forward Elements and the DEVCOM Global Technology Office to better align the international community with the Army's basic research portfolio.

Several of the ARO personnel returned in FY20 as their temporary assignment overseas concluded. Future positions will be filled as the slated positions are vacated. The international research areas, the corresponding aligned Branch, and the locations where the International Program Managers are stationed are listed below:

- Energy Transport and Storage; Chemical Sciences; Tokyo, Japan
- Human Dimension; Life Sciences; London, United Kingdom
- Innovation in Materials; Materials Science; London, United Kingdom
- Network Science and Intelligent Systems; Network Sciences; London, United Kingdom
- Quantum-Scale Materials; Physics; Tokyo, Japan
- Synthetic Biology; Life Sciences; Tokyo, Japan

University Research Initiative (URI) Program

The URI program is managed by PMs in the Tri-Service research offices (ARO, AFOSR, and ONR), and oversight comes from the Basic Research Office of OUSD(R&E). PMs have significant flexibility and discretion in how the individual projects are monitored, while OUSD(R&E) is responsible for the overall direction.

MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI) PROGRAM

The MURI program supports research efforts that require a large and highly collaborative multidisciplinary research team. This process can ultimately hasten the transition of basic research findings to practical applications and help to train students in science or engineering in areas of importance to the DoD. Therefore the MURI program supports teams whose research efforts intersect with more than one traditional discipline. These awards are typically funded at $1.25M per year for three years with an option for two additional years. The efforts are expected to promote eventual transition to Army applications by enabling rapid research and development (R&D) breakthroughs. Selection of Army research topics and the eventual awards are reviewed and approved by OUSD(R&E) under a formal acquisition process. The full list of all ARO-managed MURI efforts that were active in FY20 are described in Chapter 4.

Eight proposals were selected to be the new starts for the FY20 MURI program. The corresponding MURI topic and ARO topic author(s) (and Branch) are listed followed by the selected proposal, lead principal investigator (PI), and lead organization:

Adaptive and Adversarial Machine Learning

ARO topic author(s): Dr. Purush Iyer (Computing Sciences)
Selected proposal: Robust Concept Learning and Lifelong Adaptation Against Adversarial Attacks
Lead PI and organization: Dr. Insup Lee, University of Pennsylvania

Axion Electrodynamics beyond Maxwell's Equations

ARO topic author(s): Dr. Joe Qiu (Electronics) and Dr. Marc Ulrich (Physics)
Selected proposal: Implementation of Axion Electrodynamics in Topological Films and Devices
Lead PI and organization: Dr. Norman Peter Armitage, Johns Hopkins University

Engineering Endosymbionts to Produce Novel Functional Materials

ARO topic author(s): Dr. Micheline Strand (Life Sciences) and Dr. Chakrapani Varanasi (Materials Science)
Selected proposal: Endosymbiont Control and Enhancement of Leafhopper Brochosomes
Lead PI and organization: Dr. Jeffrey Barrick, University of Texas at Austin

Information Exchange Network Dynamics

ARO topic author(s): Drs. Derya Cansever and Edward Palazzolo (Network Sciences)
Selected proposal: A Multimodal Approach to Network Information Dynamics
Lead PI and organization: Dr. Cedric Langbort, University of Illinois at Urbana-Champaign

Mathematical Intelligence: Machines with More Fundamental Capabilities

ARO topic author(s): Dr. Joseph Myers (Mathematical Sciences) and Dr. Sara Gamble (Physics)
Selected proposal: Toward Mathematical Intelligence and Certifiable Automated Reasoning: From Theoretical Foundations to Experimental Realization
Lead PI and organization: Dr. Arthur Jaffe, Harvard University

Quantum State Engineering for Enhanced Metrology

ARO topic author(s): Dr. Paul Baker (Physics) and Dr. Joe Qiu (Electronics)
Selected proposal: Robust Entanglement-Enhanced Metrology with Atoms and Solid-State Spins
Lead PI and organization: Dr. Monika Schleier-Smith, Stanford University

Solution Electrochemistry without Electrodes

ARO topic author(s): Dr. Robert Mantz (Chemical Sciences)
Selected proposal: Plasma-Driven Solution Electrochemistry
Lead PI and organization: Dr. Peter Bruggeman, University of Minnesota, Twin Cities

Stimuli-Responsive Mechanical Metamaterials

ARO topic author(s): Dr. Samuel Stanton (Mechanical Sciences) and Dr. Dawanne Poree (Chemical Sciences)
Selected proposal: Triggering Outstanding Properties via Mechanical Adaptive Topologies (TOPMAT): Towards Dynamically Self-Amplifying Omniphoric Multiscale Metamaterials
Lead PI and organization: Dr. Nicholas Boechler, University of California, San Diego

The following seven topics were selected in FY20 and constitute the ARO portion of the FY21 MURI BAA.
The corresponding ARO PM authors (and Branch) are also listed:

Anomalous Dipole Textures in Engineered Ferroelectric Materials

ARO topic author(s): Dr. Chakrapani Varanasi (Materials Science)

Cyber Autonomy through Robust Learning and Effective Human/Bot Teaming

ARO topic author(s): Dr. Cliff Wang (Network Sciences) and Dr. MaryAnne Fields (Computing Sciences)

Highly Heterogeneous Meta-Macrostructures Created via Fine-Particle Interactions

ARO topic author(s): Dr. Julia Barzyk (Mechanical Sciences) and Dr. Michael Bakas (Materials Science)

Novel Mechanisms of Neuro-Glio Bio-Computation and Reinforcement Learning

ARO topic author(s): Dr. Derya Cansever (Network Sciences) and Dr. Frederick Gregory (Life Sciences)

Quantum Network Science

ARO topic author(s): Dr. Sara Gamble (Physics) and Dr. Derya Cansever (Network Sciences)

The Same is Different: Integrating Multiple Phenomena in Single Materials

ARO topic author(s): Dr. Marc Ulrich (Physics) and Dr. Chakrapani Varanasi (Materials Science)

Tunable Dilute Anion III-Nitride Nanostructures for Stable Photocatalysis

ARO topic author(s): Dr. Robert Mantz (Chemical Sciences) and Dr. Michael Gerhold (Electronics)

PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE) PROGRAM

The PECASE is the highest honor bestowed by the Army to extramural scientists and engineers at the outset of their independent research careers. The award recognizes investigators who show exceptional potential for leadership at the cutting edge of fundamental basic research. Awarding of the PECASE is based on two important criteria: (1) innovative research at the frontiers of science and technology that is relevant to the mission of the Army, and (2) community service demonstrated through scientific leadership, education, and outreach. Each award averages $200K per year for five years.

The 2015, 2016, and 2017 PECASE awardees were announced by the White House and funded as new start projects in FY19. The 2018 PECASE nominees are awaiting White House approval to officially begin as PECASE candidates. Rather, the 2018 PECASE nominees were funded in FY19 as Army Early Career Award for Scientists and Engineers (ECASE) awards. At the time of publication, the 2019 and 2020 PECASE nominees have not been announced.
Active PECASE Awardees and Nominees are listed by PI and organization with nominating ARO PM and Branch:

2015 PECASE Awardees

- Dr. Dhruv Batra, Georgia Institute of Technology; Dr. Purush Iyer, Computing Sciences
- Dr. Joseph Checkelsky, Massachusetts Institute of Technology; Dr. Marc Ulrich, Physics
- Dr. Phillip Christopher, University of California. Riverside; Dr. Robert Mantz, Chemical Sciences
- Dr. Jinglin Fu, Rutgers University–Camden; Dr. Stephanie McElhinny, Life Sciences

2016 PECASE Awardees

- Dr. Gordon Wetzstein, Stanford University; Dr. Hamid Krim, Computing Sciences
- Dr. Jenny Suckale, Stanford University; Dr. Julia Barzyk, Mechanical Sciences
- Dr. Percy Liang, Stanford University; Dr. Purush Iyer, Computing Sciences
- Dr. Yuji Zhao, Arizona State University; Dr. Michael Gerhold, Electronics

2017 PECASE Awardees

- Dr. Steven Brunton, University of Washington; Dr. Matthew Munson, Mechanical Sciences
- Dr. Jeff Thompson, Princeton University; Dr. Sara Gamble, Physics
- Dr. Domenic Forte, University of Florida; Dr. Cliff Wang, Network Sciences
- Dr. Katharine Tibbetts, Virginia Commonwealth University; Dr. James Parker, Chemical Sciences

2018 ECASE Awardees (PECASE Nominated)

- Dr. Bo Zhen, University of Pennsylvania; Dr. Michael Gerhold, Electronics
- Dr. Lauren Zarzar, The Pennsylvania State University; Dr. Dawanne Poree, Chemical Sciences
- Dr. Ehsan Hoque, University of Rochester; Dr. Edward Palazzolo, Network Sciences
- Dr. Jerome Fox, University of Colorado Boulder; Dr. Stephanie McElhinny, Life Sciences

STEM HIGHLIGHT

PECASE Awardees

Cutting-edge research highlights from recent awardees

Dr. Steven Brunton

James B. Morrison Endowed Career Development Professor in Mechanical Engineering; University of Washington

Project Title: Uncovering Nonlinear Flow Physics with Machine Learning Control and Sparse Modeling
Mechanical Sciences Branch (Program Manager: Dr. Matthew Munson)

Dr. Steven Brunton was awarded a PECASE in 2019 to develop new techniques that advance the modeling and control of complex fluid flows. Both the modeling and control of complex fluid flows have been difficult to achieve because of the strong nonlinear and multiscale physics inherent to systems where these flows emerge. This leads to scenarios where the governing equations needed for robust precision and control of the model have not yet been quantified.

To overcome these challenges, Dr. Brunton proposed to couple a new computational framework recently developed by his research group—sparse identification of nonlinear dynamics (SINDy)—with machine learning techniques to parse out the equations that govern even the most complex systems. The implications for the modeling framework are far-reaching, ranging from complex climate patterns, to the stability of financial markets. With the substantial time and resources afforded by the PECASE, there is potential to facilitate the interdisciplinary application of these novel techniques, ultimately leading to revolutionary new understandings that will enable future Army capabilities.

Dr. Luke Zettlemoyer

Professor; University of Washington

Project Title: Weakly Supervised Learning for Scalable Semantic Parsing
Computing Sciences Branch (Program Manager: Dr. Purush Iyer)

Dr. Luke Zettlemoyer was awarded a PECASE to advance natural language research by developing a new framework for computationally translating the underlying meaning of natural language sentences. This research is required to streamline how humans interact with computers, especially for applications like training simulations, robotic dialogue systems, and even telehealth. In recent years, significant progress had been made to develop algorithms capable of distilling the structure and context from natural language sentences. However, the technology was calibrated to small, isolated sentences, and scaling up to more complex domains was limited.

To advance the current capabilities, Dr. Zettlemoyer proposed to leverage, perhaps, the richest resource for natural language phrases: the Internet. By training algorithms on data harvested directly from the Internet, Dr. Zettlemoyer's group is developing a learning model capable of assigning meaning to sentences based on contextual information gleaned from elsewhere in the dataset. For example, the word "right" could be interpreted in different ways based on the context within the sentence. This novel framework has the potential could revolutionize the scale and fidelity of automated learning systems, enabling seamless human–computer communication.

For more information, check out Dr. Iyer's "Semantic Parsing using Deep Neural Networks" Success Story in Chapter 3!

Dr. Jerome Fox

Assistant Professor; University of Colorado Boulder

Project Title: Analysis and Design of Nonlinear Processing and Emergent Behavior in Biocatalytic Networks
Life Sciences Branch (Program Manager: Dr. Stephanie McElhinny)

Dr. Jerome Fox was awarded an ECASE in 2018 (PECASE pending White House approval) focused on unraveling the chemical pathways and relationships that enable multi-enzyme biological systems to function. The rate and structure of the metabolic pathways that produce specific biomolecules are controlled by enzymes that catalyze chemical reactions. Unfortunately, these systems are difficult to model because the nonlinear effect of multi-enzyme pathways is poorly constrained.

To overcome this research challenge, Dr. Fox proposed to develop experimental and computational methods that examine the design rules and structures that enable multi-enzyme systems to perform complex, nonlinear operations. Dr. Fox aims to systematically examine multi-enzyme metabolic pathways in vitro to quantify the mechanistic detail and synergistic effects of enzymatic cooperation. While Dr. Fox's team is using the fatty acid pathway of *E. coli* as a model system to build and validate this novel approach, this research aims to elucidate the biochemical basis of information processing, stability in dynamic environments, and the "low-power" complexity of living systems to design adjustable biochemical systems.

For more information, check out Dr. McElhinny's "Tuning the Output of Biochemical Pathways using Enzymes with Overlapping Functions" Success Story in Chapter 3!

DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

The DURIP supports the purchase of equipment that augments current university capabilities or develops new capabilities to achieve cutting-edge defense research. In FY20, the Army awarded 47 grants totaling $10M, with an average award of $217K.

University Affiliated Research Centers (UARCs)

The UARCs are strategic, Army-sponsored, DoD-designated research organizations at universities. The UARCs were formally established in May 1996 by OUSD(R&E) to advance DoD long-term goals by pursuing cutting-edge basic research and also maintain core competencies in specific domains beneficial to the DoD. Collaborations among the UARCs and the educational and research resources available at the associated universities can enhance the ability of the UARCs to meet the long-term goals of the DoD.

ARO is the primary sponsor for two UARCs and co-manages a third:

- The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT)
- The Institute for Collaborative Biotechnologies (ICB), located at the University of California, Santa Barbara, with MIT and the California Institute of Technology (Caltech) as academic partners
- The Institute for Creative Technologies (ICT), located at the University of Southern California. In contrast to the ISN and ICB, the ICT is co-managed between ARO and DEVCOM SC, where ARO is responsible for managing basic research efforts and DEVCOM SC is responsible for managing applied efforts

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs

Congress established the SBIR and STTR Programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government sponsored R&D. The purpose of these programs is to (1) stimulate technological innovation, (2) use small business to meet federal R&D needs, (3) foster and encourage participation by socially and economically disadvantaged small business concerns in technological innovation, and (4) increase private sector commercialization of innovations derived from federal R&D, thereby increasing competition, productivity, and economic growth. The STTR Program has the additional requirement that small businesses must partner with universities, federally funded R&D centers, or other nonprofit research institutions to develop and transition ideas from the laboratory to the marketplace.

The SBIR and STTR Programs are overseen by OUSD(R&E). Numerous organizations participate in the DoD's SBIR Program including the Army, Navy, Air Force, DARPA, SOCOM, DTRA, Missile Defense Agency (MDA), National Geospatial Intelligence Agency (NGA), and Chemical Biological Defense Program (CBD). The Army-wide SBIR Program is managed at DEVCOM Headquarters, which enables ARO to participate in both the Army-wide SBIR Program as well as SBIR Programs supported by other organizations across the DoD. The Army-wide STTR Program is managed by ARO. The STTR Program at ARO coordinates participation of nine Army components and commands, and invests in all Army Modernization Priorities. In addition to ARL's participation through ARO, other participating components include DEVCOM AvMC, DEVCOM AC, DEVCOM C5ISR, DEVCOM CBC, DEVCOM SC, DEVCOM GVSC, USACE, and USAMRDC.

Each year, the SBIR and STTR Programs develop a set of topics that represent the DoD's anticipated technology needs. Subject-matter experts at ARO often participate in this process by developing topics for publication in the DoD SBIR and STTR BAAs. Small businesses can then submit proposals to specific topics listed in the BAAs, which are competitively selected for funding. The SBIR and STTR Programs fund proposals through a three-phase process. Phase I is the point of entry into the program and involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Phase II represents a major R&D effort, culminating in a well-defined deliverable prototype (i.e., a technology, product, or service). Phase II awardees are competitively selected from Phase I awardees who submitted a Phase II proposal. Phase II awardees may then be selected to receive additional funds as an invited Subsequent Phase II or Phase II Enhancement (SBIR only), or via the Commercialization Readiness Program (SBIR only). Phase III represents the commercialization of the product.

In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets.

ARO FY20 SBIR AND STTR TOPICS

The following ARO SBIR topics were published in an FY20 SBIR BAA.
The lead topic author (who serves as the topic PM) and corresponding Branch are listed with each topic:

- Fieldable Decontamination System for Sensitive Equipment, Dr. Dawanne Poree, Chemical Sciences
- Expeditionary Technology Search (xTechSearch) Dual-Use Technologies to Solve Challenging Army Problems, Dr. Paul Baker, Physics
- Mid-Wave Infrared PIC-Based Coherent Beam Combining, Dr. Michael Gerhold, Electronics
- Scalable Process for Novel Nanomaterials with Infrared Filtering Properties, Dr. Dawanne Poree, Chemical Sciences
- Probabilistic Genotyping Software for Mixture Deconvolution of Next Generation Sequencing Data, Dr. Stephanie McElhinny, Life Sciences
- On-Site Formate Production, Dr. Robert Mantz, Chemical Sciences

The following ARO STTR (Army STTR) topics were published in an FY20 STTR BAA.
The lead topic author and corresponding Branch are listed with each topic:

- A Revolutionary RF Circuit Simulator for New Electronic Design and Analysis Capabilities, Dr. James Harvey, Electronics
- 300W Low-Temperature SOFC Army Power Sources, Dr. Robert Mantz, Chemical Sciences
- Photonic Accelerators for Artificial Neural Networks, Dr. Michael Gerhold, Electronics
- Cryo-CMOS Integrated Circuits, Dr. Joe Qiu, Electronics
- Virtual Off-Road Simulator for Teams of Bots and Autonomous/Conventional Wheeled/Tracked Vehicles, Dr. Joseph Myers, Mathematical Sciences
- Actuation for Human-Scale Dynamic Whole-Body Manipulation, Dr. Joseph Myers, Mathematical Sciences
- Physical Monitoring Techniques to Improve Warfighter Performance, Dr. Frederick Gregory, Life Sciences
- Three-Dimensional Microfabricated Ion Traps for Quantum Sensing and Information Processing, Dr. Sara Gamble, Physics
- Additive Manufacturing of Thermally Cured Thermoset Polymers, Dr. Dawanne Poree, Chemical Sciences
- Cost Effective Synthesis of Linear Ring Opening Metathesis Polymers, Dr. Dawanne Poree, Chemical Sciences
- Reducing COVID-19 Mortality by Reducing Post-Hyperimmunity Period Immune Suppression, Dr. Micheline Strand, Life Sciences

ARO FY20 SBIR AND STTR PHASE II CONTRACT AWARDS

The following ARO SBIR topics were selected for Phase II contracts in FY20.
The lead topic author and corresponding Branch are listed following each topic title:

- Nanostructured Electrode Materials for Enhanced Biological Charge Transfer, Dr. Stephanie McElhinny, Life Sciences
- Producing Novel Biosynthetic Therapeutics from Extreme Microbiomes, Dr. Robert Kokoska, Life Sciences
- An Adaptively Covert, High Capacity RF Communications/Control Link, Dr. James Harvey, Electronics
- Robust Wideband Full Duplex Radios, Dr. Robert Ulman, Computing Sciences
- Solid Oxide Fuel Cell (SOFC) Power System, Dr. Robert Mantz, Chemical Sciences

The following ARO STTR (Army STTR) topics were selected for Phase II contracts in FY20.
The lead topic author and corresponding Branch are listed following each topic title:

- Additive Manufacturing Feedstock Designed for Uniform Printing of Metallic Builds, Dr. Michael Bakas, Materials Science
- Carbon Nanotube Based Monolithic Millimeter-Wave Integrated Circuits, Dr. Joe Qiu, Electronics
- Diffusiophoresis for Water Purification, Dr. Matthew Munson, Mechanical Sciences
- Deep Ultraviolet Light Sources for Water Purification and Surface Sterilization, Dr. Michael Gerhold, Electronics
- Resource Sharing Platforms for Improved Operational Logistics, Dr. Purush Iyer, Computing Sciences
- Effective Human Teaming Supported by Social Sensing, Dr. Edward Palazzolo, Network Sciences
- Wavelet-Based Adaptive Antenna Systems, Dr. Joseph Myers, Mathematical Sciences
- Mitigation of Ransomware, Dr. Cliff Wang, Network Sciences
- Software Tools for Scalable Quantum Validation and Verification, Dr. T. R. Govindan, Physics
- Hybrid Nano-Bio-Electronic Odor Detector, Dr. Frederick Gregory, Life Sciences
- Disablement of Vehicles and/or Remote Weapon Stations in an Urban Environment, Dr. Joe Qiu, Electronics
- Robust High-Performance Laser Sources for Scalable Quantum Technology, Dr. T. R. Govindan, Physics
- Cell-Free Screening System for Genetically-Derived Small Molecule Biosensors, Dr. Stephanie McElhinny, Life Sciences

ARO FY20 SBIR SUBSEQUENT PHASE II CONTRACT AWARDS

The following ARO SBIR topics were selected for Subsequent Phase II contracts in FY20.
The lead topic author and corresponding Branch are listed following the topic title:

- Very High Dynamic Range RF Two Tone Measurement Instrument and Sensor, Dr. Joe Qiu, Electronics
- Coherent Beam Combining of Mid-IR Lasers, Dr. Michael Gerhold, Electronics

ARO FY20 SBIR SEQUENTIAL PHASE II CONTRACT AWARDS

The following ARO SBIR topics were selected for Sequential Phase II contracts in FY20. The lead topic author and corresponding Branch are listed following the topic title:

- Micro Weather Sensor Auxiliary Ceilometer, Dr. Elizabeth King-Doonan, Chemical Sciences
- Lyophilized Canine Plasma Sequential Phase II, Dr. Robert Mantz, Chemical Sciences

ARO FY20 STTR SUBSEQUENT PHASE II CONTRACT AWARDS

The following ARO STTR (Army STTR) topics were selected for Subsequent Phase II contracts in FY20.
The lead topic author and corresponding Branch are listed following each topic title:

- Inferring Social and Psychological Meaning in Social Media, Dr. Joseph Myers, Mathematical Sciences
- Freeze Casting of Tubular Sulfur Tolerant Materials for Solid Oxide Fuel Cells, Dr. Robert Mantz, Chemical Sciences
- Acoustically/Vibrationally Enhanced High Frequency Electromagnetic Detector for Buried Landmines, Dr. Marc Ulrich, Physics
- Quantification Model and Systems for Assessing and Developing Resilient Wireless Communication Operation, Dr. Cliff Wang, Network Sciences
- Scientific Data Management via Fast Dynamic Summarization, Dr. Joseph Myers, Mathematical Sciences
- High Performance Armor via Additive Advanced Ceramics, Dr. Michael Bakas, Materials Science
- Method for Locally Measuring Strength of a Polymer-Inorganic Interface During Cure and Aging, Dr. Dawanne Poree, Chemical Sciences

ARO FY20 STTR PHASE III CONTRACT AWARDS

The following ARO STTR (Army STTR) topics were awarded Phase III contracts in FY20. The lead topic author and corresponding Branch are listed following the topic title:

- Development of Comprehensive Biothreat Identifier—Zeteo Threat Agent Detection System (zTADS), Dr. Dawanne Poree, Chemical Sciences
- ID/IQ for SOCOM Engineering Analysis and Support, Dr. Stephen Lee, ARO Senior Research Scientist
- Lithium Ion/Super Capacitor Hybrid System, Dr. Robert Mantz, Chemical Sciences
- Wavelet-Based Adaptive Antenna Systems, Dr. Joseph Myers, Mathematical Sciences
- Rapid Detection and Identification of Biological Events, Dr. Dawanne Poree, Chemical Sciences

Historically Black Colleges and Universities and Minority-Serving Institutions (HBCUs/MIs) Program

ARO (CORE) HBCUs/MIs PROGRAM

Academic institutions classified as HBCUs/MIs may submit proposals to the core ARO BAA, as for any other institution, and are evaluated and selected according to the same evaluation criteria and process established for all proposal submissions to the ARO Core Program BAA. In FY20, ARO supported 104 agreements with HBCUs/MIs —39 of which were new agreements in FY20—receiving over $26.5M in FY20 core funding.

The core ARO HBCUs/MIs research grants awarded in FY20 are listed, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific Branch:

- Nanoscale Study of Quantum Criticality in Single Protein Molecules, Dr. Stuart Lindsay, Arizona State University; Dr. Stephanie McElhinny, Life Sciences
- Quantum Biology Studied by TEM, Dr. John Spence, Arizona State University; Dr. Stephanie McElhinny, Life Sciences
- Aberration Corrected Scanning Transmission Electron Microscope at the University of California, Santa Barbara, Dr. Susanne Stemmer, University of California, Santa Barbara; Dr. Albena Ivanisevic, Electronics
- Creating and Imaging Topological States in Two-Dimensional Materials, Dr. Brian LeRoy, University of Arizona; Dr. Joe Qiu, Electronics
- Radical Artificial Intelligence for Multiphase Environmental Systems, Dr. Ann Marie Carlton, University of California, Irvine; Dr. Elizabeth King-Doonan, Chemical Sciences
- Organically Controlled Crystal Growth and Phase Selection in Ecologically Diverse Ultrahard Biocomposites, Dr. David Kisailus, University of California, Irvine; Dr. Stephanie McElhinny, Life Sciences
- A Switch Controlling Biomolecular Reconfiguration: Tunably Controlled Calibrated Assembly, Dr. Daniel Morse, University of California, Santa Barbara; Dr. Stephanie McElhinny, Life Sciences
- Subsurface Biogeochemical Processes in Coastal Wetlands—Impacts on Water Quality, Dr. Adina Paytan, University of California, Santa Cruz; Dr. Elizabeth King-Doonan, Chemical Sciences
- Human-Agent Teaming on Intelligence Tasks, Dr. Susannah Paletz, University of Maryland, College Park; Dr. Edward Palazzolo, Network Sciences
- Quantum Optics of Correlated Systems, Dr. Mohammad Hafezi, University of Maryland, College Park; Dr. Marc Ulrich, Physics
- Facilitating the Survival and Development of Novel Ideas in Collaborative Innovation, Dr. Jared Kenworthy, University of Texas at Arlington; Dr. Edward Palazzolo, Network Sciences
- Desert Seismology: Linking Weather Saltating Particles and Dryland Geomorphology to the Ambient Seismic Environment, Dr. Julien Chaput, University of Texas at El Paso; Dr. Julia Barzyk, Mechanical Sciences
- Lattice-Matched Large-Area CdZnTe Virtual Substrates and Water-Soluble Liftoff Technology for High Performance HgCdTe Photodetectors, Dr. Yong-Hang Zhang; Arizona State University, Dr. Michael Gerhold, Electronics
- Robustness Increases Variability: A Fundamental Law of Biology, Dr. Steven Frank, University of California, Irvine; Dr. Virginia Pasour, Mathematical Sciences
- Resolving the Dynamic Interactions in the Urban Boundary Layer, Dr. Prathap Ramamurthy, City College of New York; Dr. Julia Barzyk, Mechanical Sciences
- Developing Aciniform Spider Silk Biomaterials with Unique Structural Transitions and Properties, Dr. Gregory Holland, San Diego State University Research Foundation; Dr. Stephanie McElhinny, Life Sciences

- Foundations of Deep Learning, Dr. Pierre Baldi, University of California, Irvine; Dr. Hamid Krim, Computing Sciences
- Private Information Retrieval Over Networks, Dr. Sennur Ulukus, University of Maryland, College Park; Dr. Cliff Wang, Network Sciences
- Transient Multistate Nanoparticle Assemblies Enabled by Orthogonal Dissipative Assembly Pathways, Dr. Taylor Woehl, University of Maryland, College Park; Dr. Dawanne Poree, Chemical Sciences
- Strong Correlations Meet Quantum Optics, Dr. Victor Galitski, University of Maryland, College Park; Dr. Paul Baker, Physics
- Edge-Based Machine Intelligence Architecture for In-Situ Video Processing using Binarized Neural Networks, Dr. Yu Bai, CSU Fullerton Auxiliary Services Corporation; Dr. MaryAnne Fields, Computing Sciences
- Trusted Federated Learning Algorithms in Adversarial Environments, Dr. Anna Scaglione, Arizona State University; Dr. Hamid Krim, Computing Sciences
- Graphical Games and Distributed Reinforcement Learning Control in Human-Networked Multi-Group Societies, Dr. Frank Lewis, University of Texas at Arlington; Dr. Derya Cansever, Network Sciences
- Hiding Radical Speech in Plain Sight: Covert Identity Signaling on Social Media, Dr. Paul Smaldino, University of California, Merced; Dr. Lisa Troyer, Life Sciences
- Controlling Nano-Structure Formation by Hydrodynamic Instability, Dr. Shunji Egusa, University of North Carolina at Charlotte; Dr. Matthew Munson, Mechanical Sciences
- Discovering Fundamental Laws Governing Prokaryotic Adaptation in Surface-to-Surface Transitions Using Data-Driven Inverse Modeling, Dr. Enoch Yeung, University of California, Santa Barbara; Dr. Virginia Pasour, Mathematical Sciences
- Understanding the Interplays of Mechanical and Chemical Interactions at the Molecular Interfaces of Multifunctional Bio-/Nano- Materials, Dr. Travis Shihao Hu, California State University, Los Angeles; Dr. Evan Runnerstrom, Materials Science
- CUR Decomposition and Clustering Applications, Dr. Keaton Hamm, University of Arizona; Dr. Joseph Myers, Mathematical Sciences
- Control, Optimization and Transmission Problems for Nonlocal PDEs, Dr. Mahamadi Warma, University of Puerto Rico, Rio Piedras Campus; Dr. Joseph Myers, Mathematical Sciences
- Single-Shot Ultra-Short Pulse Holographic Imaging of Dense Fuel Sprays, Dr. Derek Dunn-Rankin, University of California, Irvine; Dr. Ralph Anthenien, Mechanical Sciences
- Real Time Imaging System to Study Vital Sub-Cellular Organelles, Dr. Peter Burke, University of California, Irvine; Dr. Albena Ivanisevic, Electronics
- Probing Nonequilibrium Phonon-Magnon Coupling in Emerging Functional Materials with Femtosecond Transient Thermal and Spin Grating Spectroscopy, Dr. Bolin Liao, University of California, Santa Barbara; Dr. Chakrapani Varanasi, Materials Science
- Automated Cell Segmentation, Tracking and Quantitative Analysis: Mathematical Methods and Algorithms, Dr. Sokratis Makrogiannis, Delaware State University; Dr. Joseph Myers, Mathematical Sciences
- MWIR and LWIR Time-Resolved Photoluminescence System, Dr. Yong-Hang Zhang, Arizona State University; Dr. Michael Gerhold, Electronics
- The Effects of Specific Emotions on Ambiguous Decision Making, Dr. David Matsumoto, San Francisco State University; Dr. Lisa Troyer, Life Sciences
- Ultra-High-Speed Secure Quantum Communications, Dr. Ivan Djordjevic, University of Arizona; Dr. Derya Cansever, Network Sciences
- NTO's Degradation under Environmentally Relevant Conditions: DFT Study, Dr. Jerzy Leszczynski, Jackson State University; Dr. Elizabeth King-Doonan, Chemical Sciences
- Workshop on Assured Autonomy, Dr. Ramalingam Chellappa, University of Maryland, College Park; Dr. MaryAnne Fields, Computing Sciences
- 27th Conference on Current Trends in Computational Chemistry, Dr. Jerzy Leszczynski; Jackson State University, Dr. Elizabeth King-Doonan, Chemical Sciences

PARTNERED RESEARCH INITIATIVE (PRI) PROGRAM

The PRI Program was established as the next phase of what was previously known as the Partnership in Research Transition (PIRT) Program, which ended in FY16. The focus of the PRI Program is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army by bringing competitively selected HBCUs/MIs research teams into existing ARL Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances (CTAs). The CTAs and CRAs are large collaborative centers focused on developing and transitioning research in Army critical areas. In FY20, ARL's PRI Program for HBCUs/MIs continued funding four projects totaling $1.6M through the CTA/CRA consortia.

The CRA and CTA program and PRI topics supported in FY20 are listed, with the lead PI, collaborating institution, and cooperative agreement manager (CAM) is also listed for each topic:

Cyber Security CRA

PRI Topic: Defeating the Dark Triad in Cybersecurity Using Game Theory Integrated into Cybersecurity
Lead PI and organization: Dr. Christopher Kiekintveld, University of Texas at El Paso
CAM: Dr. Michael Frame

Multiscale Modeling of Electronic Materials (MSME) CRA

PRI Topic: Material Design Under Uncertainty
Lead PI and organization: Dr. Yanyan He, New Mexico Institute of Mining and Technology
CAM: Dr. Meredith Reed

Materials in Extreme Dynamic Environments (MEDE) CRA

PRI Topic: Tailoring Mg-Alloy Systems through Composition/Microstructure/Severe Plastic Deformation for Army Extreme Dynamic Environment Applications
Lead PI and organization: Dr. Jagannathan Sankar, North Carolina Agricultural and Technical State University
CAM: Dr. Sikhanda Satapathy

Cognition and Neuroergonomics (CaN) CTA

PRI Topic: Reliability of Neural Activity as an Assay of Cognitive State
Lead PI and organization: Dr. Jacek Dmochowski, City College of New York
CAM: Dr. Jon Touryan

DoD RESEARCH AND EDUCATIONAL PROGRAM (REP) FOR HBCUs/MIs

ARO has administered the REP on behalf of OUSD(R&E) since 1992. Under this program, qualifying institutions are able to submit proposals to compete for basic research grants. The REP aims to enhance research capabilities of HBCUs and MIs and strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

In FY20, 40 grants totaling $25.4M were made to 10 unique HBCUs and 21 unique MIs. The REP HBCUs/MIs research grants awarded in FY20 are listed, with the project title followed by the PI and performing organization:

- Unraveling Exciton Dynamics in Van der Waals Heterostructures for Optoelectronic and Photonic Applications, Dr. Gang Lu, California State University, Northridge
- Stabilizing and Recovering Polymeric Nanoscale Assemblies Utilizing Dynamic Covalent Bonds, Dr. Ishrat Khan, Clark Atlanta University
- Synthesis and Characterization of Novel Inorganic Optical Crystalline Materials, Dr. Jie Ling, Claflin University
- Synthetic Carbohydrate Receptors: Tools for Exploring and Exploiting the Most Complex Recognition in Biological Materials, Dr. Adam Braunschweig, City University of New York
- Ultra-High Precision Sensing of Isotopic Signatures using Mid-Infrared (Dual) Frequency Comb Spectroscopy, Dr. Mohammad Khan, Delaware State University
- Quantifying Complexity to Advance the Discovery and Design of Next Generation Smart Materials, Dr. William Oates, Florida A&M University
- Towards Light-Weight Composites for Defense Applications: Engineering Structure Dynamics and Rheological Properties of Functional Inks, Dr. Subramanian Ramakrishnan, Florida A&M University
- Deception-Based Security of IOBT Networks Using Intelligent Hybrid Honeypots and Game Theory, Dr. Imadeldin Mahgoub, Florida Atlantic University
- ACE: Autonomous Conformity Evaluation of Tensor Data by Means of Novel L1-Norm Principal Component Analysis, Dr. Dimitris Pados, Florida Atlantic University
- Investigation of Coastal Boundary Layer Characteristics Including Ducting Severe Storm Intensification & Aerosol Properties, Dr. Michael McCormick, Hampton University
- Aluminum Metal-Organic Frameworks Based on Metalloporphyrins and Sorption of Archetypal Organosulfur Compounds, Dr. Alexandr Samokhvalov, Morgan State University

- Manifold Segmentation and Deep Convolutional Networks, Dr. Ali Sekmen, Tennessee State University
- Understanding Roles of Flow Surface and Microbe Phenotype on Formation and 3D Architecture of Shear Resistant Biofilms with Integrated Microfluidics and Mesoscale Experimentations, Dr. Jian Sheng, Texas A&M University-Corpus Christi
- Investigation of Upper Ocean Physics and Air-Sea Interaction over the Indian Ocean and Maritime Continent, Dr. Toshiaki Shinoda, Texas A&M University-Corpus Christi
- Studies on the Mechanical Behavior of Woven Hybrid Fiber Reinforced Polymer Nanocomposites Subjected to Marine Environmental Conditions, Dr. Mahesh Hosur, Texas A&M University-Kingsville
- Ultrawide Bandgap Hetero-Structures: Growth Characterization and Modeling, Dr. Ravi Droopad, Texas State University
- Heterogeneous Integration of Diamond and Ultrawide-Bandgap Semiconductors for Fundamental Phonon and Electron Transport Studies, Dr. Edwin Piner, Texas State University
- Analyzing Migration Patterns from Central America Using Natural Language Processing and Machine Learning, Dr. Javier Osorio, University of Arizona
- Development of Sapphire Based Integrated Microwave Photonics, Dr. Aboozar Mosleh, University of Arkansas at Pine Bluff
- Functionally Integrated Materials via Additive Manufacturing, Dr. Julie Schoenung, University of California, Irvine
- A Hybrid Computational/Experimental Approach to Tuning the Specificity of Chemokine Inhibitors, Dr. Patricia Liwang, University of California, Merced
- Combinatorial Discovery of Metallic Systems with Superior Magnetic Transport Properties, Dr. Richard Wilson, University of California, Riverside
- Patterning Atomic-Scale Quantum Systems with DNA Origami, Dr. Ania Jayich, University of California, Santa Barbara
- Probing Driven Quantum Gases and Enhancing Professional Development Pathways at a Minority-Serving Institution, Dr. David Weld, University of California, Santa Barbara
- Secure and Resilient Design of Internet of Battlefield Things, Dr. Hamid Sadjadpour, University of California, Santa Cruz
- Highly Compressible Shock-Laden Turbulent Reacting Flows for Hypersonics, Dr. Kareem Ahmed, University of Central Florida
- Mechanism of O_2-dependent Nitramine Degradation by a Heme Enzyme, Dr. Jonathan Caranto, University of Central Florida
- Multilayered Protective Biomimetic Coatings from Sustainable Chitin and Chitosan, Dr. Alamgir Karim, University of Houston
- Proactive Defensive Techniques for Deception-Based Attacks, Dr. Arjun Mukherjee, University of Houston
- Compositional Testing of Network Protocols for Attacks, Dr. Lenore Zuck, University of Illinois at Chicago
- Development of Multifunctional Flexible Piezoelectric Materials for MEMS Applications, Dr. Nathan Jackson, University of New Mexico
- A Novel Model to Improve Neural Performance During Oxygen Deprivation, Dr. Joseph Santin, University of North Carolina at Greensboro
- Experimental and Numerical Investigation of Grain Shape Effects on Littoral Sediment Dynamics and Transport of Munition Constituents, Dr. Sylvia Rodriguez-Abudo, University of Puerto Rico, Mayagüez Campus
- Defect States in Time and Space Modulated Lattices, Dr. Hamidreza Ramezani, University of Texas Rio Grande Valley
- A Fast and Effective Sensitivity and Uncertainty Quantification Method for Additively Manufacturing Metals, Dr. Harry Millwater, University of Texas at San Antonio
- Optical Control of Charge and Energy Transfer in Molecular Wires, Dr. Kirk Schanze, University of Texas at San Antonio
- Understanding the Processing-Microstructure-Property Relationships of Additively Manufactured Parts during Direct Metal Laser Sintering Processes: Multi-Scale Modeling and Experimental Characterization, Dr. Jiajun Xu, University of the District of Columbia
- Using NMR Techniques to Find the Correlation of Spin Fluctuation Behavior to Superconductivity of the Iron Chalcogenide $Fe_{1+\varepsilon}Te_{0.5}Se_{0.5}$, Dr. Rosa Cardenas, University of the Incarnate Word
- Autonomous Control for Unmanned Vehicles, Dr. Michael Frye, University of the Incarnate Word
- Event Detection for Streaming Analytics: An Intelligent Mathematical Paradigm, Dr. Kun Zhang, Xavier University of Louisiana

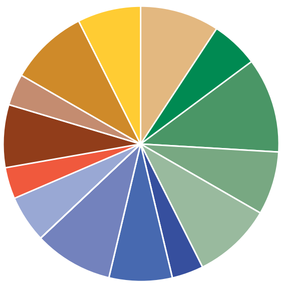
Education Outreach Program

NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The DoD NDSEG Fellowship Program is a Tri-Service research office (ARO, AFOSR, and ONR) program administered by AFOSR, designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and intend to pursue a doctoral degree in a scientific discipline of interest to the military. The NDSEG Fellowship lasts for three years and provides full tuition, a monthly stipend, a travel budget for professional development, and health insurance.

NDSEG Fellows are selected following a merit-based evaluation of the applicant's academic records, recommendations, GRE scores, and technical applications. ARO PMs serve as reviewers for applications and mentors for selectees in their areas of expertise. For a peek into the NDSEG Mentorship Program, check out the STEM highlight on the following page!

In FY20, ARO selected 54 NDSEG Fellows, who began their fellowships in fall 2021 (Figure 1).



Aeronautical and Astronautical Engineering **5**	Computer and Computational Sciences **5**
Biomedical Engineering **3**	Electrical Engineering **3**
Biosciences (includes Toxicology) **6**	Geosciences **2**
Chemical Engineering **4**	Materials Science and Engineering **4**
Chemistry **5**	Mathematics **2**
Civil Engineering **2**	Mechanical Engineering **5**
Cognitive, Neural, and Behavioral Sciences **5**	Physics **4**

Total Number of Fellows: 54

Figure 1. NDSEG Fellows Selected in FY20, by Scientific Discipline

HIGH SCHOOL APPRENTICESHIP PROGRAM (HSAP) AND UNDERGRADUATE RESEARCH APPRENTICESHIP PROGRAM (URAP)

The HSAP and URAP are managed by the Army Educational Outreach Program (AEOP) STEM Outreach Office at DEVCOM Headquarters and administered by ARO.

The HSAP funds the STEM apprenticeships of promising high school juniors and seniors to work in university-structured research environments under the mentorship of ARO-sponsored PIs or their senior research staff. In FY20, HSAP awards provided 32 students with research experiences at 20 universities in 16 states and 1 territory. Five of the universities were HBCUs/MIs. ARO invested approximately $46K into the FY20 HSAP effort, and the AEOP contributed matching funds.

The URAP funds STEM apprenticeship of undergraduates to work in research groups under the mentorship of ARO-sponsored PIs or their senior research staff. In FY20, URAP awards provided 50 students with research experiences at 32 universities in 22 states and 1 territory. Seven of the universities were HBCUs/MIs. ARO invested approximately $148K into the FY20 URAP effort, and the AEOP contributed matching funds.

STEM HIGHLIGHT

Experiences

HSAP and URAP Summer Apprenticeship Program

2020 was a year like no other. Despite some initial challenges and setbacks, the AEOP was able to provide virtual apprenticeships for 90% of the high school and undergraduate students who submitted applications to the summer program. Here is what the students had to say:

"I enjoyed my experience with the Apprenticeship Program! I was able to learn a lot including, writing, presenting, and other technical STEM skills. I was able to communicate with my mentor every day, sometimes multiple times a day, and participate in professional meetings with other researchers. I also got the chance to present my research at a symposium and conference. I was given a lot of opportunities through the Apprenticeship Program to learn and develop skills."
–URAP Participant

"I was very satisfied with the Apprenticeship Program. Even though the program has ended, I am able to continue the work that I have begun with my mentor and further the research done in the field."
–HSAP Participant

"I enjoyed this program and very much appreciate the opportunity! I wish I would've been able to participate in the program in the lab itself and conduct research but exposure to quantum programming was beneficial too. I am looking forward to exploring my options next year and in college to remain involved in AEOP."
–URAP Participant

For more information, check out Ms. Ardouin's "Ensuring Summer Apprenticeship Programs in the Midst of COVID-19 Restrictions" Success Story in Chapter 3!

LOCAL AND VIRTUAL OUTREACH

The Education Outreach Program also works with local organizations to coordinate opportunities for ARO to participate in community STEM events. These programs reach kindergarten through high school students, teachers, the general public, and other researchers through activities including career fairs, informal science activities, workshops, and seminars.

Although public health concerns surrounding the COVID-19 pandemic precluded many outreach events from occurring in person in FY20, it did provide ARO with an opportunity to participate in a number of virtual events both locally and nationwide. The following is a snapshot of the outreach opportunities that ARO participated in during FY20:

- STEM Fests: ARO joined STEM RTP, a nonprofit organization that facilitates STEM outreach and mentoring opportunities for underrepresented minorities during their 2020 Expos/Fairs. In November 2019, ARO PMs volunteered as speed mentors to an estimated 180 middle and high school students. When the spring STEMFest went virtual in April 2020, ARO PMs also served as mentor panelists to inspire the next generation of STEM professionals.
- Career Fairs: ARO participated in career fairs at local middle schools and North Carolina State University in FY20. ARO PMs and staff volunteered to discuss aspects of their own STEM careers within DoD and explain how important STEM careers are to the country.
- RTP180: This is a monthly event series organized by STEM RTP where speakers are selected to present their research interests to members of the local community. In FY20, Dr. Sara Gamble (Physics Branch) and Dr. Stephen Lee (Senior Research Scientist, Interdisciplinary Sciences) were both selected to discuss the current trends and cutting-edge research in their fields.
- AEOP Virtual STEMinar Series: When the HSAP and URAP summer apprenticeships became virtual, AEOP organized their STEMinar Series—where speakers, including Senior Research Scientists from ARO, were able to engage with HSAP participants on topics ranging from tips on college attendance, STEM entrepreneurship, applying for other DoD STEM opportunities, and the latest in scientific discovery.

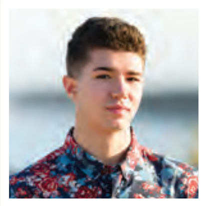
Scientific Services Program (SSP)

The SSP was established by ARO in 1957, and is currently administered and managed for ARO through the Edmond Scientific Company (headquartered in Alexandria, Virginia). This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analytical services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academics working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any science and technology area of interest to the government.

The SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, materials science, and military personnel recruitment/retention. In FY20, 11 new SSP tasks were awarded with 5 modifications to the scope and/or funding of ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY20 new SSP tasks is provided in Table 1.

Sponsoring Organization	SSP Tasks
DEVCOM	
ARL	2
Soldier Center	1
Total: DEVCOM	**3**
OTHER U.S. ARMY	
Combined Arms Support Command (CASCOM)	1
Headquarters, U.S. Department of the Army, Deputy Chief of Staff (HODA DCS)	1
Program Executive Office for Simulation, Training and Instrumentation (PEO STRI)	1
Total: Other U.S. Army	**3**
OTHER DoD	
Defense Logistics Agency (DLA)	1
Strategic Environment Research and Development Program (SERDP)	1
Defense Health Agency (DHA)	2
Joint Program Executive Office Armaments and Ammunition (JPEO A&A)	1
Total: Other DoD	**5**
TOTAL FY20 New SSP Tasks	**11**

Table 1: Summary of agencies participating in the FY20 SSP



STEM HIGHLIGHT

NDSEG Fellowship Mentor-Mentee Interviews

ARO Polymer Chemistry Program Manager, Dr. Dawanne Poree, and her NDSEG Fellow, Dorian Bruch, share their thoughts on mentoring and the NDSEG Fellowship.

Please tell us a little bit about yourself. Where did you go to school? What are your research interests? What is your current position?

Dawanne (mentor): I am a native of New Orleans, Louisiana. I attended Nicholls State University for my undergrad, where I received a B.S. in Chemistry. I then did my graduate studies at Tulane University, where I received a Ph.D. in Chemistry, with a concentration in Polymer Science. As my research training was in synthetic polymer chemistry, my personal research interest is the design of novel synthetic techniques that allow for making polymers previously unattainable. Currently, I am a Chemist at ARO, managing the Polymer Chemistry extramural basic research portfolio.

Dorian (mentee): I am currently a second year Ph.D. student in Chemical Engineering at the California Institute of Technology. I received my B.S. in Chemical Engineering from the University of California, Santa Barbara in 2019. I am most interested in the field of thermodynamics and statistical mechanics. Previously, I've worked on modeling the nucleation of the order–disorder transition of diblock copolymers using self-consistent field theory in tandem with the string method. Currently, I have been focusing on modeling electrolyte and polyelectrolyte solutions in the presence of charged surfaces, as well as calculating interaction forces between charged surfaces.

What did you learn about your mentor or mentee professionally or scholastically that surprised/impressed you?

Dawanne (mentor): I was immediately struck by how self-aware Dorian is. He seemed to know exactly what he wanted to get out of this mentor–mentee relationship, and provided me with very specific ways I could help him through his graduate school journey. This tells me that Dorian is very driven and goal-oriented, which will serve him scholastically as well as professionally.

Dorian (mentee): I was surprised to learn that my mentor also worked with block copolymers, and it was impressive to hear that she used them for potential biomedical applications, such as using star block copolymers as transdermal drug delivery agents.

How do you hope to, or how did you, benefit from mentoring?

Dawanne (mentor): Anytime I can share an experience that helps someone else in their journey is a benefit to me. It is my hope that I can impart some wisdom from my journey through STEM graduate training and now as a STEM professional that will help make his journey easier and hopefully even enjoyable.

How do you hope to, or how did you, benefit from mentorship?

Dorian (mentee): The mentorship has, and I hope will continue, to provide me with professional advice, such as seeking job opportunities in my area of expertise and receiving feedback on my work, as well as general life advice, such as work–life balance as a graduate student.

Can you share any advice for students thinking about a graduate degree or career in a STEM field?

Dawanne (mentor): Embarking on a career/degree in a STEM field is not for the faint of heart. There will always be setbacks and failures (that's why it's call "RE"search). Don't let the failures define you. Embrace them. See them as opportunities for growth.

Dorian (mentee): My biggest piece of advice is that when you're applying to/deciding on a graduate school, you should thoroughly think about which professor you would like to work with. Your professor will have a large impact on your graduate school experience.

Thinking about past mentorship experiences, how have they shaped your approach to mentorship?

Dawanne (mentor): My prior mentors have been sounding boards on my roughest days, while also providing me the space to navigate the journey and make the choices and decisions that were right for me. This has absolutely shaped how I approach mentorship. I don't want my decisions and how I chose to navigate the process to be prescriptive of how my mentee should approach his journey. I just want to be there to offer a sound ear and perspective, whenever it's needed.

Summary of ARO Funding and Program Actions

Below is a summary of funding and program actions for FY20. The majority of the reported statistics refer only to mission-driven funds (not externally leveraged funds).

FY20 Funding Actions

PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify how the proposed research could better align with program vision and Army needs. Approximately one-third of the white papers received by ARO PMs from academic institutions are submitted as formal, full proposals.

Notes: The numbers to the right refer to new-start proposals in the basic research categories: SI, STIR, ECP/YIP, HBCUs/MIs, MURI, and DURIP. Data does not include support by externally leveraged funds. Data Source: ARO New Starts in FY2020 Report (19 January 2021).

2,076
White papers received in FY20

624
Proposals received in FY20

381
Total new agreements awarded following a competitive peer-review process

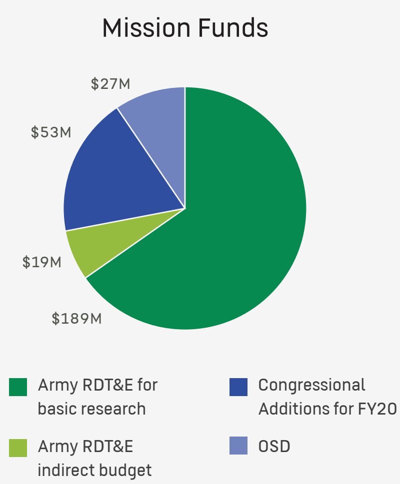
79
Agreements awarded to HBCUs/MIs

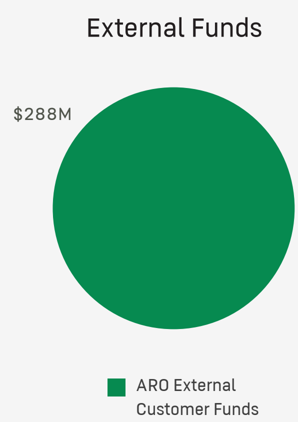
12
Agreements awarded through the Early Career Program

Where ARO Funding Comes From

ARO is funded primarily by the Army and OSD, which totaled $289 million in FY20. The majority of funding that ARO receives from the Army is categorized as either 6.1 basic research or R&D basic research, and is carried in the Army's Research, Development, Test & Evaluation (RDT&E) account. Additional sources of Army funding are provided by Congressional Additions. The amount and intended use of Congressional Additions can vary year to year. ARO is also in the unique position to leverage funds from other stakeholders including (but not limited to) DARPA, DRTA, ONR, AFOSR, USACE, and USAMRDC.

Notes: Totals may not add due to rounding. Data Source: ARO General Fund Enterprise Business System (GFEBS) Status of Funds Report (30 September 2020).

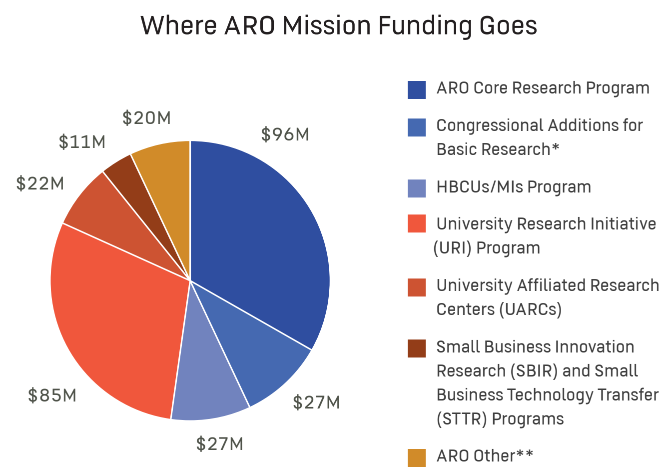




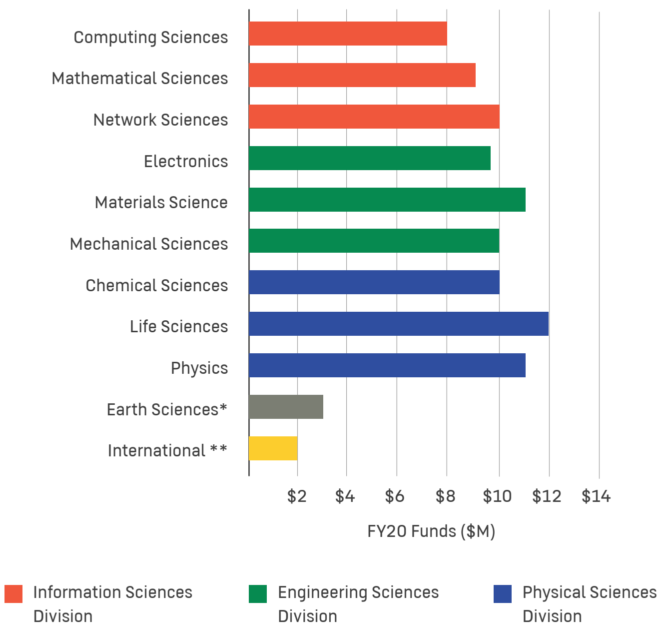
Where ARO Funding Goes

ARO pursues a variety of different research programs and initiatives that have unique objectives and eligibility requirements (as described above). The ARO Core Research Program is the largest extramural funding program and is organized as a function of scientific discipline (Branch). The other ARO program and initiatives also tend to align with the Core Research Program scientific disciplines as PMs participate in topic formulation, proposal selection, and award monitoring throughout the organization.

Notes: Totals may not add due to rounding. *Congressional Additions for Basic Research are typically set aside for specific programs and/or projects. **ARO Other comprises funds set aside for ARO general and administrative support, the Minerva Research Institute, and the Board of Army RDT&E, Systems Acquisition, and Logistics (BARSL) activities. Data Source: ARO GFEBS Status of Funds Report (30 September 2020).

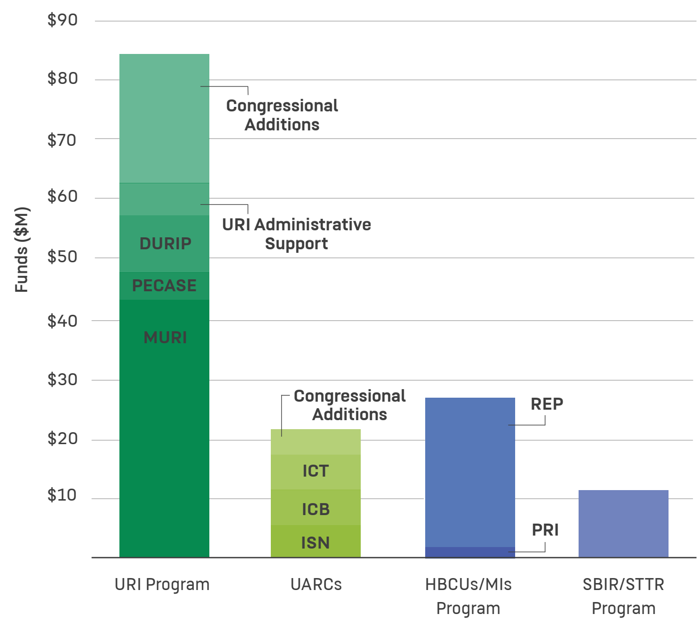


Core Research Program: Scientific Disciplines



Notes: Totals may not add due to rounding. *Earth Sciences is split between the Chemical Sciences and Mechanical Sciences Branches. **The International Program supports six topic areas: Energy Transport and Storage, Human Dimension, Innovation in Materials, Network Science and Intelligent Systems, Quantum-Scale Materials, and Synthetic Biology. Data Source: ARO GFEBS Status of Funds Report (30 September 2020).

ARO Special Programs



Notes: Totals may not add due to rounding. Data Source: ARO GFEBS Status of Funds Report (30 September 2020).

How ARO Funding is Awarded

Of all of the agreements that are currently active, 83% percent of support from ARO goes to institutions of higher education. The remaining awards go to private industry, including small businesses and non-profit institutions; federal, state, and local governments; and federally funded research centers. In FY20, 508 individual organizations received support from ARO, 82 of which were designated as HBCUs/MIs.

For agreements that started in FY20, ARO awarded most funds as grants (71%) and cooperative agreements (7%). Cooperative agreements are specialized grants that are used to enable substantial involvement from DoD agencies. The remaining funds were awarded as contracts, which are used to acquire products and services for DoD use.

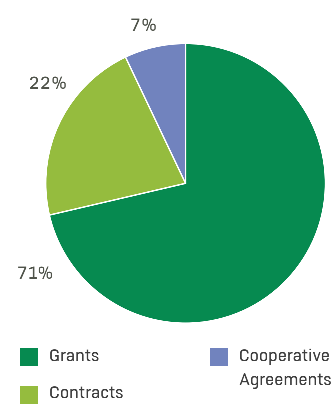
508
Organizations received ARO funding in FY20

249
U.S. institutions of higher education

82
HBCUs/MIs

40
International institutions of higher education

Agreements Awarded in FY20



Notes: Totals may not add due to rounding. Data does not include people supported by externally leveraged funds. Source: ARO New Starts in FY2020 Report (19 January 2021)

ARO's Commitment to Capacity Building for the Nation

The Nation must be prepared for a world dependent on science, technology, engineering, and mathematics (STEM) capabilities. Investment in U.S. institutions, researchers, and students from all sectors of society ensures that the Nation will maintain technological overmatch. Further, identifying and supporting international organizations at the cutting edge of S&T ensures that the United States remains the leader in the global scientific enterprise.

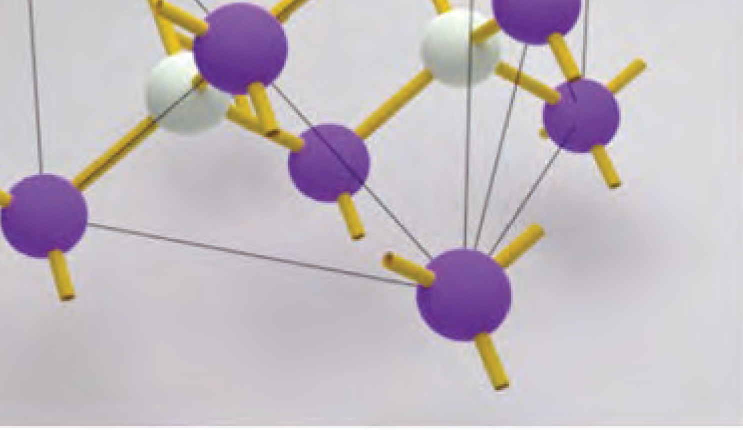
5,627 People directly supported by ARO
Researchers, postdoctoral fellows, technicians, and students

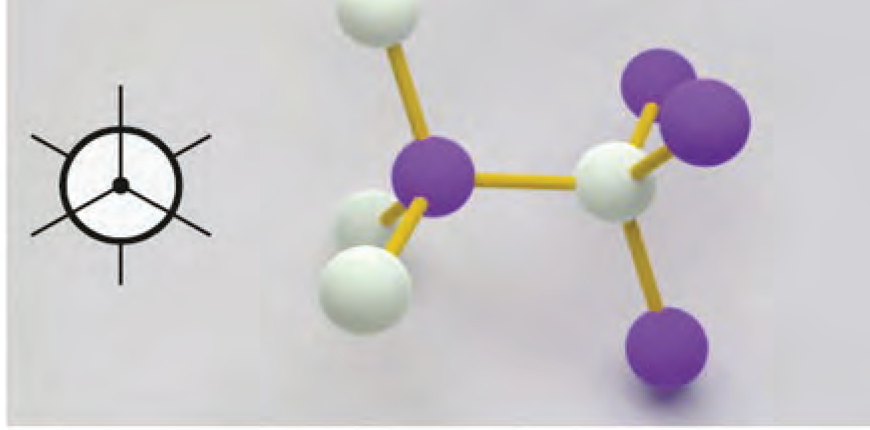
2,977
Faculty and other professionals supported by ARO

2,650
Students supported by ARO (high school through graduate)

82
High School and Undergraduate Apprenticeships supported by ARO

Notes: Data does not include people supported by externally-leveraged funds. Data Source: ARO Research Performance Progress Report (RPPR) Participant Counts by FY Report (12 January 2021). High School and Undergraduate Apprenticeship and NDSEG Fellowship data courtesy of the Education Outreach Program.

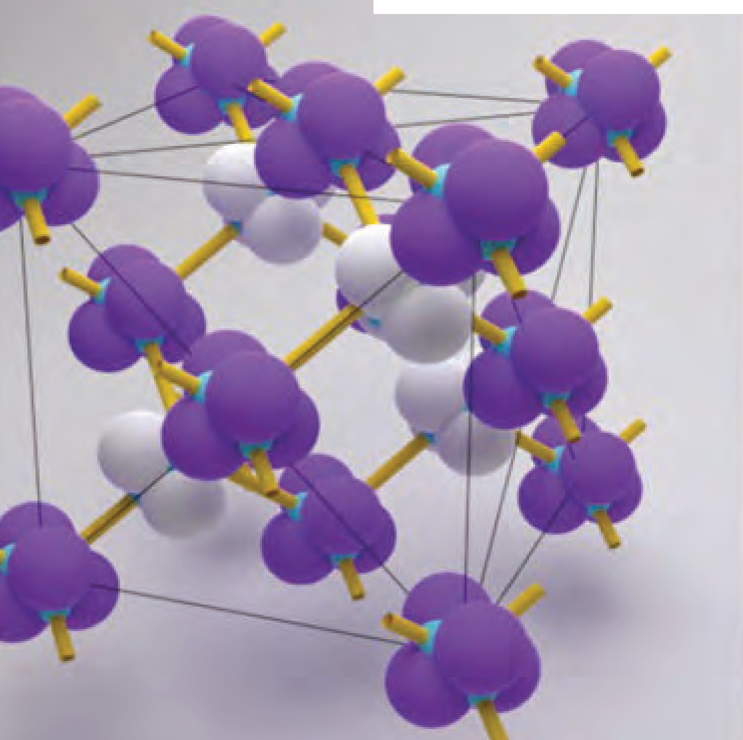


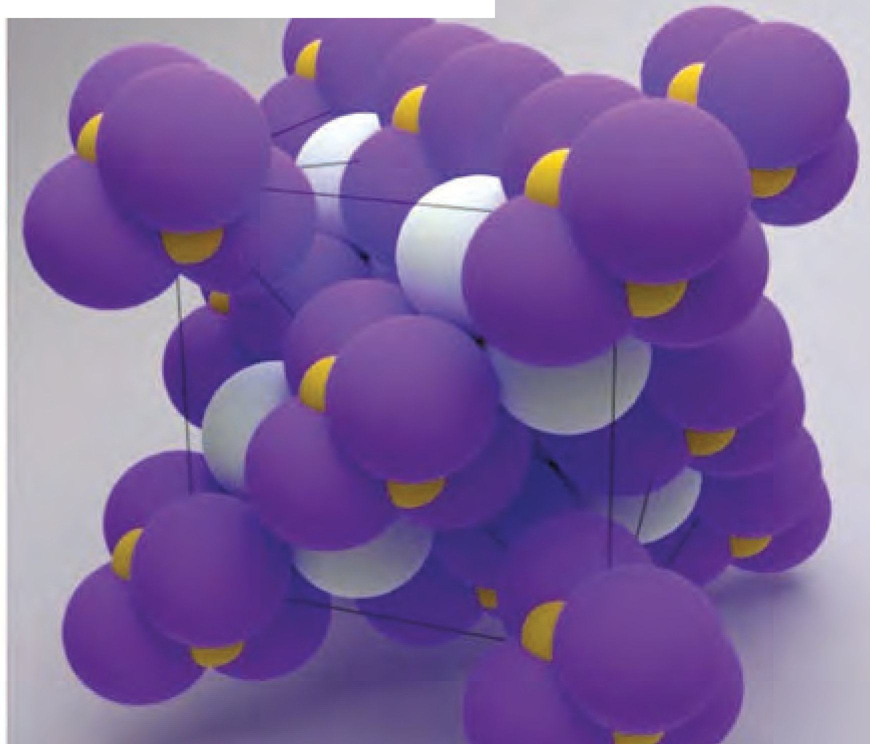


Chapter 3
Success Stories

This chapter provides a brief summary of the ARO Success Stories in FY20, organized by ARO Division, Branch, and the associated Program Manager (PM) or other ARO staff. Each success story represents fundamental studies that will also impact one or more of the ARL Competencies.

This background image is from "Diamond and Beyond: New Horizons in Colloidal Self-Assembly" on page 49.





Success Story	Associated ARO PM/POC	Pg #	SEM	PE&QS	MIS	BBS	HCS	NS&CS	TE	WS	EMSS	ES	MS
Engineering Sciences Division													
Three-Dimensional Multifunctional Neural Interfaces for Cortical Spheroids and Engineered Assembloids	Ivanisevic, Harvey (retired)	33				●	●						
Photo-Responsive Organic Molecules for All-Optical Switches	Ivanisevic, Harvey (retired)	35				●	●						
Novel Metamorphic Heterostructures with Indium Arsenide Antimonide (InAsSb)-Based Strained-Layer Superlattice Absorbers	Paskova, Gerhold, Clark (retired)	37				●	●						
Toward Uncooled Thermal Imaging Focal Plane Devices with Extremely High Sensitivity	Paskova, Gerhold, Clark (retired)	39		●							●		
Device Architectures for Superior Data Communications in Both Ambient and Cryogenic Environments	Gerhold	41		●	●			●					
Using Topological Physics to Overcome Integrated Photonic Circuit Challenges	Gerhold	43		●	●			●					
Rare Earth Element Material Could Produce World's Smallest Transistors	Qiu	45		●									
A New Ferroelectric van der Waals Heterojunction with Record-High Tunneling Electroresistance	Qiu	47		●									
Diamond and Beyond: New Horizons in Colloidal Self-Assembly	Runnerstrom, Prater (retired), Kiserow (retired)	49	●	●									
Materials Surface Science for Water Purification	Runnerstrom, Varanasi, Prater (retired)	51	●	●		●							
Stick-Slip Dynamics in Granular Materials	Cole, Stepp, Barzyk	53	●						●				●
High-Pressure Mechanochemistry	Cole, Stepp	55	●						●				
Chief Scientist Spotlight	Stepp	57											
Novel Organic Materials with Extraordinary Functional Properties: Two-Dimensional van der Waals Metal-Organic Frameworks and Covalent Organic Frameworks	Varanasi, Poree	59		●							●		
Engineering Defects in Novel Materials for Future Quantum Information Systems	Varanasi, Gamble, Govindan, Fatemi	61		●	●						●		
Defining Printability for Additively Manufactured Alloys	Bakas, McWilliams, Jelis	63	●										
Three-Dimensional Digital Characterization of Grain Structures	Bakas, Hernandez	65	●										
Active Structures Bridging Mechanics and Computation	Stanton, Ford, Ulrich	67	●										●
Understanding and Engineering Extreme Actuation in Future Robotics	Stanton, Kokoska	69	●										●
Solid Bridging to Explain Fine-Particle Aggregation	Barzyk	71	●										●
Particle-Scale Tracking and Bulk-Scale Modeling of River Sediments	Barzyk	73	●										●
Clearing Your Head: The Mechanics of Glymphatic Waste Clearance	Munson, Gregory	75				●							
The Knotty Problem of Vortex Dynamics	Munson	77							●				●
Optical Characterization of Subsurface Reactions in Heterogeneous Materials	Anthenien	79							●	●			
Simultaneous Velocity, Temperature, and Formaldehyde Imaging to Study Ignition in High-Pressure Turbulent Jets	Anthenien	81										●	
A Nature-Inspired Library for the Design of Lightweight Impact-Resistant Materials	Ford, Anthenien	83							●	●			
Novel Optical Technique for Impact-Induced Damage Evolution in High-Strength Low-Toughness Materials	Ford, Anthenien	85	●						●				
International Division													
The Ear as a Route to Augmented Soldier Performance and Machine Integration	Gregory	87					●						
Bringing Consistency to Laser Powder Bed Fusion Processing of Metal Alloys	Harvey, Bakas, Fife, Varanasi	90	●										

Success Story	Associated ARO PM/POC	Pg #	SEM	PE&QS	MIS	BBS	HCS	NS&CS	TE	WS	EMSS	ES	MS
Information Sciences Division													
4D Visualization of Fire Events in Ground Vehicles	Coyle	93				●		●					
Multi-Human Multi-Robot Interactions	Coyle	95			●			●					
New Processing Module Improves Performance of Deep Neural Networks	Fields, Coyle	97					●	●					●
Redesigning Deep Neural Networks for Small Processors	Fields, Iyer	99					●	●					●
Confocal Diffusion Tomography: 3D Imaging through Scattering Media	Krim	101					●	●					
Distributed Learning for Collaborative Fusion	Krim	102						●					
Semantic Parsing using Deep Neural Networks	Iyer	104					●	●					
Fast Identification of Triangle and k-Cliques in Large Graphs	Iyer	106					●	●					
Senior Research Scientist Spotlight	West	107											
A Quantitative Approach to the Biochronicity of Circadian Rhythm, Sleep, and Neurobehavioral Performance	Pasour	110				●	●						
Role of Rapid Eye Movement (REM) Sleep in Emotional Memory Consolidation with Implications for Post-Traumatic Stress Disorder	Pasour, Gregory	112				●	●						
Multiscale Fast and Distributed Data and Statistics Summarization	Myers, Fox	114						●					
New Computational Methods for World-Class Engineering Modeling in Army Turbine Applications	Myers, Fox	116						●		●			
Statistical Topological Data Analysis	Balu, Myers	118					●			●			
Sensor Target Detection and Classification	Balu, Myers	120						●					
Quickest Detection	Lavine	122			●		●	●					
Targeted Network Sampling	Lavine	124			●		●	●					
Achieving Reliability Guarantees for Critical Systems	Wang	126			●			●					
Applying Domain Constraints for More Secure Cyber Machine Learning (ML) Systems	Wang	128			●			●					
Verifiable Reinforcement Learning in Networked Systems	Cansever	130						●					
Distributed Robust Nonconvex Optimization over Time-Varying Networks: Tradeoffs and Guarantees	Cansever	131						●					
Building Cognitive Resilience in Human–Agent Teams	Palazzolo	133			●		●	●					
Network Propagation Model Predicts Both Information and Viral Spread	Palazzolo	135			●		●	●					
Secure Wireless Communications Bounds Using Full-Duplex Communications	Ulman, Cansever	137			●		●	●					
Distributed Data Processing and Machine Learning Algorithms for Wireless Battlefield Networks	Ulman, Cansever	138						●					
Laser-Activated Plasma (LAPLAS) for Standoff Electronic Denial	Caccuitto, Gerhold, Fox	140						●					
Nonlinear RF Interference Mitigation Achieves Initial Success	Caccuitto, Qiu, Fox	142						●					
Senior Research Scientist Spotlight	Lee	143											
Low Temperature Electrochemical O_2 Pumps for Medical O_2 from Air	Fox, Parker	145	●										
Multi-Hit Performance of Small-Arms Protective Armor	Fox, Stepp	146	●							●			
Ensuring Summer Apprenticeship Programs in the Midst of COVID-19 Restrictions	Ardouin	149	●	●	●	●	●	●	●	●	●	●	●
North Carolina Agricultural and Technical State University (NC A&T) Influence on the Materials in Extreme Dynamic Environments (MEDE) Collaborative Research Alliances (CRA)	Huff	151	●										

Success Story	Associated ARO PM/POC	Pg #	SEM	PE&QS	MIS	BBS	HCS	NS&CS	TE	WS	EMSS	ES	MS
Physical Sciences Division													
Single-Particle Spectroelectrochemistry	Mantz	153										●	
Hot Electron Injection in Photocatalytic Plasmon-Resonant Nanostructures	Mantz, Parker	155										●	
Identifying Transport Mechanisms of Volatile Organic Compounds Expected to Improve Protection from Industrial or Wartime Chemical Release Events	King-Doonan, Parker	157			●		●						
Environmental Forensics for the Detection, Classification, and Transformation of Engineered Nanomaterials	King-Doonan, Mantz	159	●										
Oxygen Purification via Nanomembrane Separation	Parker, Gerhold, Fox	161		●									
New Raman Spectroscopic Method to Determine the Reliability of Solid Rocket Propellants in Real Time	Parker, Everitt, Rice	163	●										
Toward Sequence-Defined Synthetic Polymers via Engineered Translation Machinery	Poree, McElhinny	165				●							
Rapid, High-Resolution 3D Printing Using Visible Light	Poree	167	●										
Chasing Droplets: Predator–Prey Interactions	Poree, Prater (retired)	169	●										
Reactivity Descriptors of Single-Atom Catalysts	Poree	171	●										
A Protein-Based Material Capable of Rapid Self-Healing	McElhinny	173	●			●							
Tuning the Output of Biochemical Pathways Using Enzymes with Overlapping Functions	McElhinny	175				●							
Aging, Senescence, and Death: The Impact on Warfighter Readiness	Strand, Kokoska	177				●							
Mitochondrial Chromatin Accessibility	Strand	179				●							
Life on the Rocks: Microbial Survival in Desert Environments	Kokoska	181	●			●							
Resource Sharing via Microbial Fusion	Kokoska	183				●						●	
Applying Big Data to Enhance Human Visual Search Performance	Gregory	185					●						
Understanding Gut Feelings: From Gut to Brain and Back	Gregory, Pasour	187					●						
Path-Breaking Research Identifies Neurological Indicators of Dominance and Social Influence in Groups	Troyer	189				●	●						
Undetectable Vocal Spectrum Patterns Identify Emerging Influential Actors	Troyer	191				●	●						
Seconds-Scale Coherent Optical Clock	Baker	193	●	●				●					
Transverse-Field Ising Dynamics in a Rydberg-Dressed Atomic Gas	Baker	195	●	●				●					
Integrated Quantum Sensing and Control for High-Fidelity Qubit Operations	Gamble, Govindan, Stanton	197		●				●					
From Quantum Algorithms to Quantum Startups to Quantum Partnerships	Gamble, Govindan	199		●				●					
Senior Research Scientist Spotlight	Reynolds	201											
Driven Imposters	Joseph, Myers	205		●							●		
Vortex Microlaser	Joseph	207		●				●					
Rich Interactions between Topological and Magnetic States	Ulrich, Qiu	209		●									
Transition Physics Between Topological States Revealed	Ulrich	211		●									
Genetic Tuning of Magnetic Iron Oxide Nanoparticle Size, Shape, and Surface Properties in *M. magneticum*	Burgess, Kokoska	213		●		●							
Fundamental Understanding of Human Adaptive Cognition during Physical Exertion	Burgess, Kokoska	215			●		●						
Widely Tunable Compact Terahertz Gas Laser	Burgess, McConville, Everitt	217	●	●							●		
Ductile Ceramics	Burgess, McConville	219	●									●	●

BIOTRONICS PROGRAM

Program Manager
Dr. Albena Ivanisevic

Dr. Ivanisevic completed her undergraduate studies at Drake University, receiving her B.S. in Chemistry in 1996. She trained as a surface chemist at the University of Wisconsin-Madison, receiving her Ph.D. in Inorganic Chemistry in 2000.

She came to ARO in 2020 as the Program Manager for Biotronics after 18 years as a faculty member at Purdue University and North Carolina State University.

Current Scientific Objectives

1 Achieve control of the most useful material system that can be used to influence and probe cells via their bioelectronics-dependent behavior that, if successful, will enable future read-outs and actuation technologies to interrogate cellular activity, which could lead to future body-heat-powered devices to modernize Soldier lethality and advanced body implants integrated into the neural systems to augment ongoing Soldier performance.

2 Probe living cells' intrinsic bioelectric fields from the "outside" (no cell penetration) using electronic modalities that, if successful, will enable novel electrochemical sensors to track key biomarkers, which could lead to wearable body sensors and control systems for expeditionary Soldier and environmental sensors with high sensitivity and survivability in harsh conditions so Soldiers can quickly understand and react to emerging situations, thus increasing their lethality, precision, and survivability.

This success was made possible by:

Dr. Albena Ivanisevic,
Electronics Branch

Dr. James Harvey,
International Division

SUCCESS STORY

Three-Dimensional Multifunctional Neural Interfaces for Cortical Spheroids and Engineered Assembloids

This ARO initiative resulted in the creation of the first 3D structures as multifunctional neural interfaces to spheroids and as frameworks for the formation of engineered assembloids. The results create new opportunities for using human stem cell derived model tissues in fundamental studies of processes related to neuroregeneration and recovery from neurotraumatic injury.

CHALLENGE

Three-dimensional submillimeter-scale constructs of neural cells, known as cortical spheroids and organoids, are of rapidly growing importance in neuroscience research due to their ability to reproduce complex features of brain architecture, function, and organization in vitro. Despite their great potential for studying neurodevelopment, neurological diseases, and neurotraumic injury, such types of miniaturized, fragile 3D living biosystems cannot be easily examined using conventional methods for neuromodulation, sensing, and manipulation. An ideal solution would involve compliant, shape-matched multimodal platforms of cellular-scale microdevices in 3D geometries that gently envelop the spheroids/organoids as multifunctional electronic, optoelectronic, thermal, mechanical, and biochemical interfaces. Such a system, which enables 3D probing of these neural cells, would have the potential to unlock new insights into how the human brain works.

ACTION

Dr. Ivanisevic discussed the challenge with Dr. Cameron Good from the Lethality Division at ARL WMRD. Together they identified the work of Professor John Rogers from Northwestern University as particularly promising in this area. Dr. Ivanisevic reached out to Professor Rogers to discuss the research and opportunities in the field, which prompted Professor Rogers to formulate a competitive proposal focused on 3D in vitro models, rather than 2D cell cultures, of dissociated neuron cultures that more closely resemble native cell-to-cell communication and architecture.

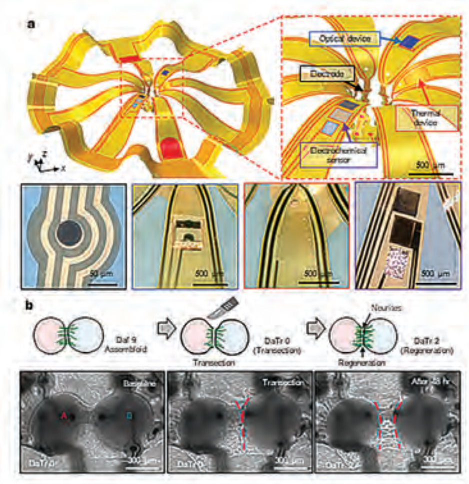


Figure 1: (A) 3D multifunctional framework as a neural interface to a cortical spheroid (Top: structure; Bottom: devices). (B) Studies of neuroregeneration of a neurite bridge between a pair of spheroids (Top: schematic illustrations; Bottom: optical micrographs). Courtesy of Professor John Rogers.

Specifically, the resulting proposal exploited ideas to yield frameworks with individually addressable combinations of components that allow for single-cell active interfaces for diverse optical, pharmacological, and electrical modes of interaction. The goal of the proposed work was to generate a comprehensive picture of how alterations in molecular pathway signaling within single cells translates to changes in cellular activity of both neurons and astrocytes at the individual cell level, and how these changes modify behavior at the network level. Professor Rogers' proposal was funded in 2020 with a three-year Single Investigator grant.

RESULT

Professor Rogers has developed a unique 3D neural interface platform that exploits multifunctional, cellular-scale microdevices in highly compliant, open-mesh network architectures with reversible, engineering control over shapes, sizes, and geometries to match organoids/spheroids of interest (Figure 1). The ability to exploit the most advanced planar electronic and optoelectronic technologies in these systems represents a key defining feature that allows advanced functionality of various types relevant to high-performance neural interfaces operating across scales that range from the subcellular, to the cellular and network levels. Use of the assembloids will reduce the amount of in vivo experiments researchers need to perform. An example of the power of these new technologies is in quantitative electrophysiological studies of neuroregeneration between lobes of transected assembloids formed from a pair of spheroids for research in neuroscience and regenerative medicine. Detailed electrophysiological studies in a setup that joins a pair of spheroids in close proximity reveal insights into processes associated with the growth, transection, and regrowth of the neurite bridge, the biological connection that forms naturally between these spheroids. Specifically, the bridge between these two spheroids regenerates and recovers over a period of days, corresponding to timescales comparable to its original formation. This model reproduces neurite regeneration in a 3D human system and provides direct electrical evidence of functional integration as well as key information for understanding neurological development and regeneration in vitro, for instance, in traumatic brain injury, axonal injury in the central nervous system, multiple sclerosis, and stroke.

WAY AHEAD

Spheroids, organoids, and assembloids have already contributed much to our understanding of neurodevelopmental disorders and neurotraumatic injury. The 3D neurotechnology platform introduced here will allow researchers to harness that potential with greater detail and efficiency than can be realized using conventional methodologies. Future opportunities include research in microfluidic networks for delivery of pharmaceutical agents and sampling of adjacent fluids, biochemical sensors for monitoring the transport of biomarkers to and from tissue surfaces, scaffolds for improving nutrient perfusion to maintain deep cells, and penetrating multifunctional probes. These 3D neural interfaces have the potential to give new insights into treating a variety of neural conditions such as traumatic brain injury and stroke.

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

Results

- Provided the first example of a 3D neurotechnology system as a functional interface to spheroids and organoids.
- Demonstrated these structures as 3D microscale frameworks for positioning multiple spheroids as precursors to complex yet deterministic assembloids.
- Studied the processes of neuroregeneration associated with transection and regrowth of a neurite bridge between a pair of cortical spheroids formed using human-induced pluripotent stem cells.

Anticipated Impact

Neuromodulation studies using 3D frameworks as interfaces to human brain organoid cultures derived from patients provides a potential path to explore effective routes to care for impaired Soldiers. Diverse 3D functional frameworks enable various studies of neurodevelopment diseases, neuroregeneration, and related therapies and rehabilitation protocols needed for Army personnel.

This success was made possible by:

Dr. Albena Ivanisevic,
Electronics Branch

Dr. James Harvey,
International Division

Citations:

He, J. *et al. Optics Express* **28**, 22462-22477 (2020).

Kovach, A., He, J., Saris, P. J. G., Chen, D. & Armani, A. M. *AIP Advances* **10** (2020).

SUCCESS STORY

Photo-Responsive Organic Molecules for All-Optical Switches

This ARO initiative resulted in the design and synthesis of a photo-responsive organic small molecule. Subsequently, as an initial application, the molecule is self-assembled on the surface of an integrated photonic circuit, creating an all-optically switchable optical filter.

CHALLENGE

Imaging techniques, like fluorescent microscopy, have transformed our understanding of the role of electric fields in governing intra- and intercellular communications, but they are being pushed to their limits. To continue to explore the inherent complexity of biological systems, which could lead to new therapeutics and diagnostics, innovative solutions for investigating bioelectric fields are needed. One promising new material system is based on light-responsive organic small molecules. These nanoscale materials interact with light in customizable ways, potentially allowing researchers to investigate cell–cell interactions and study the formation of transient subcellular structures. These new materials also have applications beyond biology such as telecommunications, energy, and imaging.

ACTION

Dr. Ivanisevic initiated discussions with Professor Andrea Armani from the University of Southern California. She proposed the idea of triggerable molecular devices for detecting and modulating bioelectric fields. Extensive communication between Dr. Ivanisevic and Professor Armani resulted in a proposal that aimed to synthesize a molecular device comprising a pair of covalently coupled electric-field-responsive small molecules. One acts as an electric-field detector and reporter, and the second acts as an electric-field modulator. The aim was that both molecules perform independently. It was proposed to study the effect of time-varying electrical defects in muscle cells (cardiomyocytes) upon their interaction with neighboring cells. These discussions culminated in a Single Investigator award in 2020.

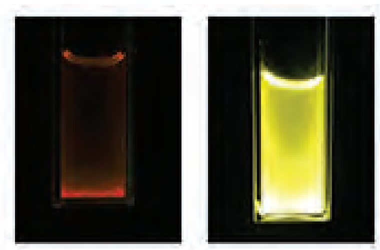


Figure 2: A synthesized light-emitting material. (Left) The material illuminated by room light. (Right) The material illuminated by 350-nm light. Similar emission is observed when the material is illuminated around 750 nm. Courtesy of Professor Andrea Armani.

RESULT

To date, efforts in Professor Armani's lab have resulted in the creation of a suite of new light-responsive materials. In initial efforts, theoretical calculations and modeling of the molecules were performed to predict their behavior, also known as a priori material design. This emerging material design approach allows for accelerated research progress and reduces the overall material cost. Subsequently, multiple groups of photo-responsive organic small molecules were synthesized, including materials that emit light for imaging (Figure 2) and materials that change their shape at the nanoscale in response to light.

To characterize the nanoscale length change, researchers demonstrated an application in telecommunications of an all-optically switchable photonic circuit, namely, an optical filter. This work involved developing surface chemistry, anchoring a single monolayer of the switchable molecules to the photonic circuit surface, and simultaneously injecting two wavelengths of light into the device (Figure 3).

> "The advantages of this method include robust attachment of a simple surface chemistry that does not change the operability or optical performance of the devices."
>
> – From He et al. (2020)

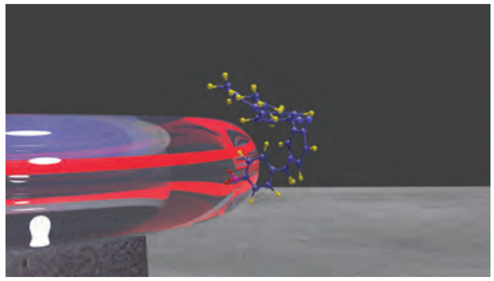
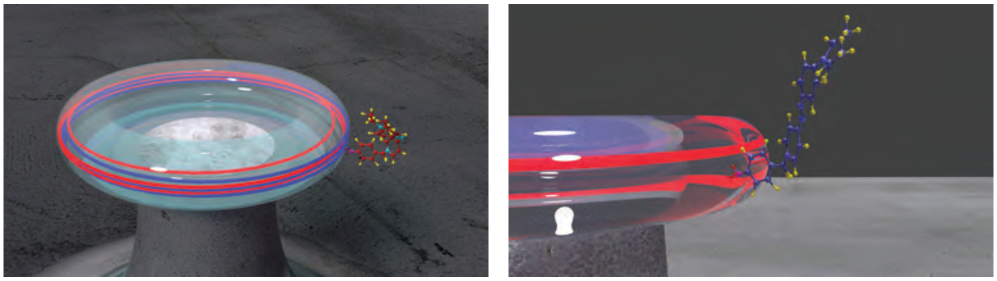


Figure 3: Rendering of the integrated optical device. The molecule is anchored on the device surface. When different wavelengths of light are injected into the device, they trigger the molecule to extend or collapse. The process is completely reversible and stable in air. Adapted from He et al.(2020).



Published in the spring of 2020, this work represents the first organic, all-optical integrated photonic circuit (He et al., 2020). It offers many advantages over the conventional approaches for fabricating switchable optical circuits, including lower power and lower heat generation. Additionally, unlike previous organic systems, due to the mechanism of action, the system is environmentally stable. Stability and response reproducibility are key criteria both in integrated photonics as well as biological imaging.

WAY AHEAD

The techniques developed are now being translated to understand the effect of nanoscale deformations of the cell membrane on bioelectric-field-based cell communications using optical imaging. Notably, this approach is noninvasive, allowing measurements to be performed without directly disturbing the cell or the surrounding cellular matrix. These findings could reveal new mechanisms of action, inspiring new approaches to prevent disease progression or providing new paths for therapeutic design.

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

Results

- Synthesized and integrated new photo-responsive organic small molecules with photonic integrated circuits.
- Demonstrated for the first time all-optical switches with an integrated photonic circuit.
- Highlighted by the American Institute of Physics (AIP) in May as a top paper in *AIP Advances* and was presented at ARL in January 2020.

Anticipated Impact

The molecular device being constructed can enable researchers to simultaneously and noninvasively modify the bioelectric field and measure the impact on the biological system as well as the individual cell. This ability will transform how researchers design experimental studies in bioelectric fields and will pave the way for discovery of ways to direct them for the purposes of improving Soldier performance.

ELECTRONIC SENSING PROGRAM

Program Manager
Dr. Tania Paskova

Dr. Paskova obtained her M.S. in Microelectronics in 1984 and Ph.D. in Physics in 1993 from Sofia University, Bulgaria. She trained as a physicist and crystal grower at Linkoping University, Sweden.

She came to ARO in 2020 as the Program Manager for Electronic Sensing Program after more than 25 years of experience in academia, industry, and government agencies.

Current Scientific Objectives

1| Develop new heterostructure designs with superior material quality and carrier transport that, if successful, will enable detectors with high quantum efficiency, high time resolution, short dead times, low noise, and ideally photon-number resolution that are anticipated to lead to unprecedented optical, thermal, and electronic warfare sensors.

2| Model and explore novel detector concept in advanced heterostructures employing metamaterials and metasurfaces in conjunction with photonics that, if successful, will enable a significantly enhanced ability to harness and direct energy toward the active sensing region and is anticipated to lead to smaller, more-efficient sensors.

This success was made possible by:

Dr. Michael Gerhold, Electronics Branch

Dr. William Clark (retired), Electronics Branch

Dr. Tania Paskova, Electronics Branch

Citations:

Suchalkin, S. *et al*. *Appl. Phys. Lett*. **116**, 032101 (2020).

SUCCESS STORY

Novel Metamorphic Heterostructures with Indium Arsenide Antimonide (InAsSb)-Based Strained-Layer Superlattice Absorbers

This ARO-funded research demonstrated short-period metamorphic indium arsenide antimonide ($InSb_xAs_{1-x}/InSb_yAs_{1-y}$) strained-layer superlattices (SLSs) with enhanced vertical hole transport in the growth direction, high optical absorption, and the possibility for effective control of the refractive index that could lead to photodetectors with significantly improved performance in the entire long-wavelength infrared (LWIR) range of 8-15 µm at temperatures above 200 K.

CHALLENGE

Remote sensing and object imaging are critical tools for maintaining situational awareness. In the 1970s using type-II superlattices (T2SLs), stacks of layers of certain materials that yielded unusual behaviors were proposed as a method for making infrared (IR) detectors, competing with the established mercury cadmium telluride (HgCdTe) ones. Since then, these sensors have been realized as commercial products. However, the published information on the fundamental absorption in T2SLs indicates insufficient understanding regarding how to control the material properties and optimize the T2SL design to employ their full potential. Filling this knowledge gap is critical for remote sensing and object imaging, considering that a large portion of photons emitted by remote objects near room temperature falls into the LWIR range of 8-15 µm.

ACTION

The unique research approach pursued by scientists from the Optoelectronics Group at the State University of New York at Stony Brook (Stony Brook),, focusing on the development of an optimized T2SL design based on metamorphic direct bandgap III-V materials (i.e., materials with at least one group III element and at least one group V element), was identified by the former Electronic Sensing Program Managers Drs. William Clark (retired) and Michael Gerhold as very promising for LWIR photodetectors. ARO supported the Stony Brook effort using both Single Investigator and Defense University Research Instrumentation Program (DURIP) grants in 2017. The DURIP grant enhanced the materials growth facilities and provided capabilities for effective production of so-called metamorphic structures on virtual substrates (VSs) (i.e., materials combinations that are not limited by the availability of an ideal substrate). The VS approach allows the material's atomic separation (lattice constant) to be a design parameter, which enables growth of bulk InAsSb with an arbitrary composition of antimony (Sb) thereby tuning the absorption wavelength. The success in growing bulk alloys was instrumental in the subsequent development of InAsSb structures with real-space periodic modulation of the arsenic (As)/Sb-ratio. This is another way of thinking of a superlattice (i.e., a structure with artificial periodic variation of the local potential). By this approach, the effective bandgap of the structure can be further reduced (≤0.1 eV) to zero and, in fact, even reach inversion, which would allow IR sensors to reach even further in the far-IR region.

The success of the III-V materials development also relied on advanced materials characterization techniques available to the team via close collaboration with ARL, as well as specifically developed at Stony Brook labs to control material quality and establish fundamental properties. Dr. Gerhold recognized the opportunity of combining the synergistic expertise in growth, characterization, and theoretical methods. While attending a forum at ARL's Center for Semiconductor Modeling (CSM) in January 2020, he identified the potential benefit of theoretical simulations for guiding the device design and encouraged the Stony Brook-ARL team to collaborate with the CSM, providing expertise in device simulations. The joint effort allowed the band structure and physical properties of the novel narrowband/gapless VS-based materials to be studied by a variety of methods, including measurements of angle-resolved photoemission, carrier lifetime, and mobility. The experimental results were also used in support of model validation by the CSM.

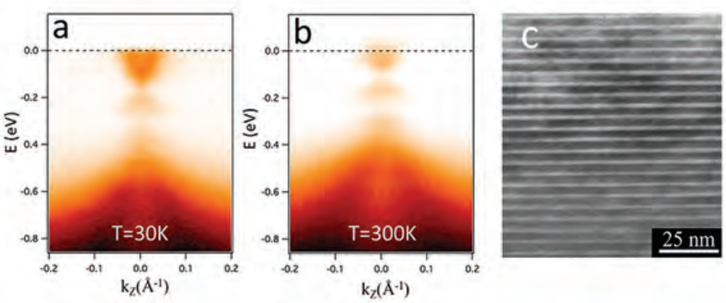


Figure 1: (A) The new material can exhibit Dirac-type anisotropic energy dispersion confirmed by angle-resolved photoemission spectroscopy. (B) With increasing the temperature from cryogenic to 300 K, the bandgap shrinks to zero (making the material "gapless") or even to negative numbers (making it an "inverted bandgap" material). (C) Transmission electron microscopy image of a cross section of $InSb_xAs_{1-x}/InSb_yAs_{1-y}$ metamorphic superlattices, showing high-quality, dislocation-free material. Adapted from Suchalkin et al. (2020).

RESULT

It was demonstrated that high-quality InAsSb alloys can be grown by molecular beam epitaxy on gallium antimonide (GaSb) substrates with gallium indium antimonide (GaInSb) compositionally graded metamorphic buffers, which help accommodation of lattice-mismatch-induced strain and avoiding defect formation. Lifting the substrate lattice constant design constraint opened up a much wider parameter space for engineering energy gaps, energy dispersion, heterobarrier offsets, and fundamental carrier recombination and scattering properties.

Using these buffers, high-quality, narrow direct gap InAsSb alloys with low temperature energy gaps as low as 90 meV have been demonstrated. This allows optically driven device operation in a very broad spectral range, spanning wavelengths from about 3 to 12 μm and reaching an even wider range at higher temperatures. The fact that the bandgap of InAsSb could reach much smaller values than had been previously thought represents a significant material discovery. This breakthrough opened up the possibility of using the III-V alloy as a substitute for HgCdTe in devices operating in the IR band.

The team also developed short-period metamorphic $InSb_xAs_{1-x}/InSb_yAs_{1-y}$ SLSs, representing a new class of quasi 3D materials with ultra-low bandgap and anisotropic carrier dispersion (Figure 1A). They also demonstrated that with increasing temperature from cryogenic to 300 K the bandgap shrinks to zero (making the material "gapless") or even to negative numbers (making it an "inverted bandgap" material; Figure 1B). Narrow gap (< 0.1 eV) InAsSb-based SLS with strong bulk-like fundamental optical absorption characteristics and enhanced hole transport have been demonstrated. High-quality heterostructures with sharp interfaces were obtained by optimization of crystal growth temperature and growth rates (Figure 1C). Moreover, low valence band offset barrier heterostructures with SLS absorbers have been developed and used for several important purposes, including measurement of minority carrier lifetime and diffusion length, demonstration of light detection, and high-speed laser beam intensity modulation.

In addition, energy gaps approaching zero and linear energy dispersion of carriers have been confirmed by magneto-optic measurements. Extension of the energy gap range down to zero and inversion of conduction and valence bands while preserving desirable bulk-like properties of $InAsSb_x/InAsSb_y$ SLSs were achieved by using a short period (2-5 nm) of modulation of the Sb composition, allowing hole tunneling with enhanced hole transport and strong fundamental absorption. Such SLSs provide a flexible platform for realizing quantum materials and developing ultra-sensitive detectors with tunable spectral characteristics.

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

Results

- Developed a new IR sensing material by using new advanced processes with higher levels of control and flexibility in III-V semiconductor crystal growth.
- Led to close collaboration with ARL ensuring continuous transition of knowledge to the Army.
- Co-published numerous papers with Army and SUNY researchers in multiple prestigious journals.

Anticipated Impact

The new approach of short-period SLSs is expected to cover the entire LWIR range up to 15 μm, critically important for high-performance thermal imaging of remote objects at near room temperatures.

WAY AHEAD

The results of the collaborative research suggest that metamorphic heterostructures with bulk and strained-layer superlattices could ultimately offer InAsSb-based absorbers with significantly improved absorption and minority hole transport that could overcome some limitations of T2SL photodetectors. The materials are also being explored for topologically enabled devices.

The ARO Electronic Sensing Program Managers Drs. Gerhold (former) and Paskova (current) recognized the importance of the growth and properties enhancement and continue to support the team to further explore the metamorphically grown superlattices with very thin layers, including the ones with a deep band inversion, as an absorber material for IR photodetectors specifically targeting extension of the quantum efficiency of the detectors in the 12-15 μm spectral range. If successful, the effort will lead to development of ultra-sensitive detectors in the very far-IR region.

This success was made possible by:

Dr. Michael Gerhold, Electronics Branch

Dr. William Clark (retired), Electronics Branch

Dr. Tania Paskova, Electronics Branch

Citations:

Lee, Y.-J., Das, A., & Talghader, J. J. *Optics Express* **28**, 5448-5458 (2020).

SUCCESS STORY

Toward Uncooled Thermal Imaging Focal Plane Devices with Extremely High Sensitivity

This ARO-funded research demonstrated a resonant-cavity pyrometer with record high detective capabilities for an uncooled device and is exploring the fundamental physics of cavity enhanced thermal detectors that can result in imaging performance able to see temperature differences that are nearly as small as 1 mK, which would enable the detection of the faintest thermal signatures possible before background fluctuation noise become a limitation.

CHALLENGE

The highest-performance IR images are used on satellites, aircraft, and other systems where the relatively large size, weight, power, and maintenance requirements of cryogenic cooling are acceptable. For the Soldier, IR performance is sacrificed for simplicity and portability. ARO-funded efforts are ongoing to close the gap between cooled and uncooled imaging with the goal of providing Soldiers with the most advanced technology platforms.

Two of the biggest limitations that prevent uncooled focal plane arrays (FPAs) from reaching the performance of their cooled counterparts are their slow speed and high noise. In principle, a very-large-area uncooled detector will operate at the theoretical radiation limit, but its enormous thermal mass will slow down measurements, making such devices unsuitable for Army needs.

Radiation noise can be reduced by absorbing only certain wavelengths of light. Such wavelength selection can be achieved using special materials or structures, but the use of a coupled infrared cavity of high quality factor, which remains a significant challenge in LWIR, would amplify multi-pass optical propagation of the infrared light, making the approach electrically tunable across large swaths of the IR spectrum. A coupled cavity requires a complex design: part of the cavity of highly transparent material needs to manipulate and direct the light into a small device region of highly absorbing material. Such a combination of high and low absorption regions would enable the detector to collect large amounts of light while remaining nimble with a fast response.

ACTION

To fulfill these requirements, the device structure must have a far higher IR absorption per unit mass than has been achieved before. With this, one can choose the smallest device mass that enables the desired imaging performance (limited by statistical thermal fluctuations), and then maximize the area of the detector so that its noise is radiation-limited. Aiming to achieve both low noise and high speed of uncooled devices, the former Electronic Sensing Program Managers Dr. Michael Gerhold and Dr. William Clark (retired) worked extensively with ARL scientists and related Defense Advanced Research Projects Agency (DARPA) programs in the area of optical and IR devices, microelectromechanical systems, and detection. Dr. Gerhold sought information on these issues in many forums from DARPA program reviews to Joint Technology Office (JTO) meetings. Dr. Clark initially identified the University of Minnesota group and in 2015 awarded Professor Joey Talghader a Single Investigator grant to develop uncooled devices that captured specific wavelengths. Based on the outcomes from this work, Dr. Gerhold recognized that overcoming issues of speed and noise required advances in device structures, which, in turn, required new materials, and funded a new research program to achieve these goals in 2018.

RESULT

At the beginning of this effort, Professor Talghader's group designed a set of experimental microbolometers to have reduced radiation noise. During the testing of the first generation of these devices, measurements showed that the radiation improvements went as expected, but no gain in performance could be seen because a parasitic noise was too high. To tackle this issue, the team changed their readout strategy from resistor to thermopile, which has no bias current and thus no appreciable noise (termed 1/f noise, or pink noise). With this and other materials changes, Professor Talghader's group was able to demonstrate uncooled LWIR detectors with a detection limit substantially higher than ever achieved before. A scanning electron microscope (SEM) image of device of this type is shown in Figure 2.

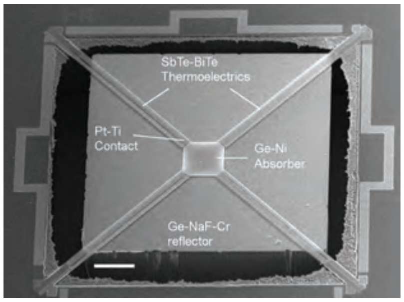


Figure 2: A SEM image of an uncooled detector of the type with the highest published detectivity. Scale bar is equal to 100 μm. Adapted from Professor Joey Talghader.

While the goal of the first program focused largely on device design advancement, further developments will require better LWIR materials, and this is the main topic of the current ARO supported research of Professor Talghader's group. Interestingly, both extremely low absorption materials and extremely high absorption materials are needed to enable the new device concepts. In this way, light can be manipulated and directed by highly transparent layers into a highly absorbing engineered sublayer of small periodic structures with low thermal mass. This gives both light efficiency and fast time constant. Diamond is theoretically one of the best low absorption materials. Using diamond, Professor Talghader's group recently demonstrated high transparency optical resonators beyond 9-mm wavelengths, a first for LWIR systems (Figure 3A). These devices and their experimental setup are shown in Figure 3B, together with some characteristic resonance transmission data (Figure 3C).

To achieve higher absorption, Professor Talghader's group has been taking a different approach. The goal is not so much to get high absolute absorption, which can be done with many materials, but rather to get high absorption (near 100%) with the smallest possible amount of material. This would allow room-temperature detectors to have a maximum area while maintaining the minimum mass necessary to meet thermodynamic requirements on temperature fluctuations. The team is designing subwavelength metastructures for which theory indicates an absorption per unit mass far lower than ever achieved before, enabling near-radiation-limited performance.

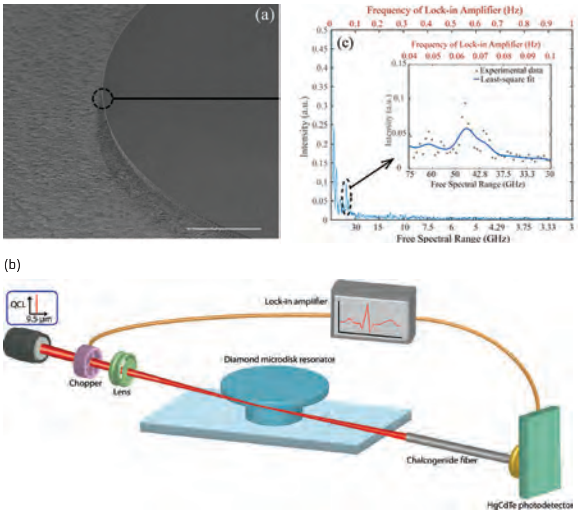


Figure 3: (A) A SEM image of a diamond micro-disk resonator structure. Scale bar is 100 μm; (B) Optical measurement setup consisting of a tunable quantum cascade laser (9–10 μm) coupled to a single-crystal diamond micro-disk. The uncoupled light was collected by a single-mode As_2Se_3 chalcogenide fiber, and was detected by an HgCdTe photodetector; (C) Fourier transform of intensity vs. wavelength plot for the first microresonator, when included in the experimental setup. Adapted from Lee et al. (2020).

WAY AHEAD

Drs. Gerhold and Paskova have continued basic research investment in Professor Talghader's group aiming to explore the fundamental physics of thermal detectors implementing both microcavities and metamaterials and validate the theoretical predictions. Combining the advances of noise reduction and maximizing absorption per unit mass, Professor Talghader's group is developing uncooled detectors able to image temperature differences that are nearly as small as 1 mK, as opposed to current technology with values more than an order of magnitude higher. If successful, this would represent uncooled devices operating near the theoretical limits set for them by statistical thermodynamics, and thus closing the gap between cooled and uncooled device performance to less than a factor of two, rather than the orders of magnitude differences today.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

Results

- Demonstrated uncooled devices with record high detectivity for a microstructure without cooling.
- Demonstrated ultra-high transparency in the LWIR cavities using diamond microresonators, displaying the highest finesse achieved for IR wavelengths greater than 9 μm.
- Published these results in a prestigious journal and was selected as the Editor's Pick for the Mid-infrared, Longwave, and Terahertz (MLT) Photonics Feature issue of *Optics Express*.

Anticipated Impact

The research is expected to contribute to development of a new thermal detector paradigms involving metamaterials and microcavities to perform at background limited levels, while eliminating the need for cooling, allowing for the development of lightweight, next-generation thermal imaging technologies suitable for the dismounted Soldier or other small platforms.

OPTOELECTRONICS PROGRAM

Program Manager
Dr. Michael Gerhold

Dr. Gerhold completed his undergraduate studies at Purdue University, receiving his B.S. in Electrical Engineering in 1992 and M.S. in Electrical Engineering in 1994. He received his Ph.D. in Electrical Engineering from the University of Michigan in 1999.

He came to ARO in 1999 as the Program Manager for Optoelectronics.

Current Scientific Objectives

1 | Explore the limits of low-energy and high-speed optoelectronics to assess ways to surpass the performance of conventional electronics or consider hybrid integrated microsystems of the two that, if successful, will enable accomplishing faster and higher-performance computing on mobile platforms with limited power supplies.

2 | Advance photonics capabilities through exploration of high-intensity radiation generation within microscale systems that, if successful, will enable chip-scale photonic light sources (from ultraviolet to mid-infrared) based upon novel materials that will enhance Army surveillance, sensing, and communications.

This success was made possible by:

Dr. Michael Gerhold,
Electronics Branch

Citations:

Wang, H.-L., Qiu, J., Yu, X., Fu, W. & Feng, M. *IEEE Journal of Quantum Electronics* **56**, 1-6 (2020).

Fu, W. *et al. 2020 IEEE Photonics Conference (IPC)* 1-2 (2020).

SUCCESS STORY

Device Architectures for Superior Data Communications in Both Ambient and Cryogenic Environments

A laser of superior transverse modal characteristics has shown promise to impact low-cost, rugged-environment military data communications as well as commercial data center applications at up to kilometer-scale links.

CHALLENGE

High-fidelity communication capabilities, especially in austere, rugged environments, are an important requirement for military operations. Semiconductor diode lasers have experienced success in both edge-emitting and vertical-cavity surface-emitting laser (VCSEL) regimes. However, these technologies have experienced roadblocks to achieving kilometer-scale optical interconnects—they cannot attain sufficiently high power levels while maintaining beam purity. Overcoming semiconductor laser power limitations can enhance Multi-Domain Operations via means of much higher data rates and longer distance communication links enabling faster decision-making and for networked sensors.

ACTION

Starting in 2013, Dr. Gerhold has made strategic investments in Professor Milton Feng's laboratory at the University of Illinois at Urbana-Champaign to enhance high-speed optical device concepts research and related measurement capabilities. Providing state-of-the-art characterization capabilities within universities accelerates the opportunity for discoveries that advance low-energy, high-speed optoelectronics. Dr. Gerhold's Defense University Research Instrumentation Program (DURIP) and Single Investigator investments have enabled Professor Feng to achieve world-record optoelectronic device speeds. In concert with these investments, Dr. Gerhold facilitated a collaboration between Professor Feng and Dr. Dennis Deppe of sdPhotonics, LLC, which has led to discoveries of opportunities to advance cryogenic computing.

RESULT

The recent advances described here shatter a long-standing scientific barrier to optical communications. This barrier is based upon the problem that occurs as one increases the size of a VCSEL in a bid to increase the power capabilities of these state-of-the-art devices. With an increase in size, the laser emits multi-lobed spatial modes. These higher-order modes limit the communication distance possible at a given data rate. The figure of merit for this fiber dispersion effect is referred to as the effective modulation bandwidth (EMB). As a result of ARO's recent investments, Professor Feng has overcome many of these challenges and has presented results with his new lasers in the leading conference on optical communications, the 2020 Optical Fiber Communication Conference, and published them in the *IEEE Journal of Quantum Electronics* (Wang et al., 2020). Additionally, Professor Feng is patenting an idea of creating an effective graded index profile he used to achieve a larger-diameter—effectively single-mode—laser.

Surprisingly, the Feng architecture is quite easily fabricated. Output power levels for single-mode operation have reached milliwatt levels, sufficient to exceed the stated 4,700-MHz*km EMB limit inherent to "OM4" fibers—the fiber commonly used for multimode optical links. Professor Feng's discoveries can, at the same data rate, extend the communication distance of these state-of-the-art fibers by an order of magnitude. Also, the patented approach does not affect the laser efficiency, reliability, or operation temperature range. The impact is thus transformative for Army systems because Professor Feng's VCSELs can be mass produced at low cost and incorporated into both multimode and possibly single-mode fiber systems. The larger core multimode systems are desirable for easier install and replacement due to larger alignment tolerance, but single-mode systems may be used in advanced systems for high-performance computing. Figure 1A shows that across a wide temperature range of operation, the novel laser designs suppress higher-order mode power by 1,000 times. Figure 1B indicates how the development single-mode VCSELs can exceed the previously stated limits thought to be inherent to OM4 fiber.

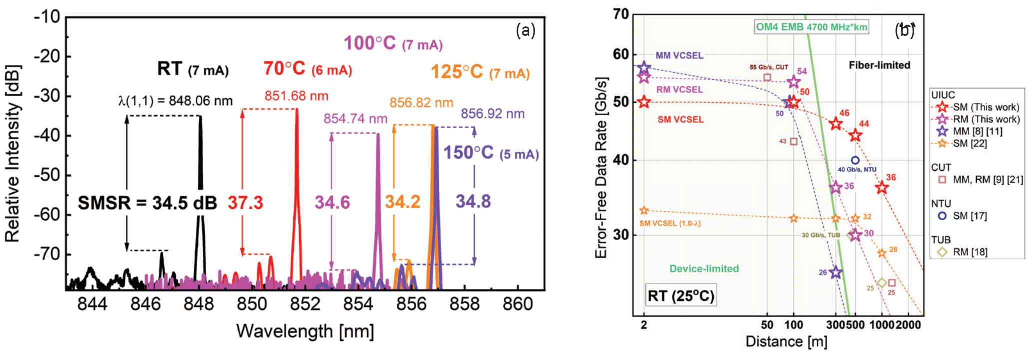


Figure 1: (A) Effectively single-mode VCSEL optical spectra measured with a side-mode suppression ratio (SMSR) of >34 dB from room temperature (RT) to 150 °C. Thirty decibels is a factor of 1,000. (B) VCSEL error-free data-rate versus distance are plotted up to 1 km at RT. Single-mode (SM) VCSELs demonstrate results beyond the fiber's inherent limits when using multimode VCSELs; see points at distances of >300 m. Adapted from Wang et al. (2020).

Dr. Gerhold also facilitated a collaboration between Professor Feng's lab and Professor Dennis Deppe of the University of Central Florida (now with his spin-off company, sdPhotonics, LLC). They jointly explored how VCSELs can solve long-standing bandwidth limitations seen in cryogenic applications, such as where focal plane arrays are cooled for high-sensitivity surveillance. Professor Feng measured sdPhotonics' designed VCSELs that performed much better than expected at these liquid-nitrogen-cooled temperatures. These lasers operated adequately at frequencies four times higher at cryogenic temperatures than they did at room temperature. Figure 2A shows one of these lasers operating at cryogenic temperatures (82.1 K, in this case) for a series of drive currents. So long as the response does not drop below a factor of 3 dB, the laser is operating profitably. This data shows that this laser can be driven up to 48 GHz and it is limited by the test setup rather than the device itself, indicating that even higher frequencies are possible. The maximum data rate for a laser is twice this operation frequency (referred to as "modulation bandwidth"). This increase opens scientific questions as to why cryogenic operation is so much faster. The lasing temperature dependence was not thought to be so dramatic, but the trends seen in Figure 2B show vast potential for high speeds with cryogenic cooling.

The measurements of both the oxide and oxide-free VCSELs (sdPhotonics' design) by Professors Feng led to a larger ARO and Intelligence Advanced Research Projects Activity (IARPA) program to explore 4K cryogenic optical links. Very-low operating temperatures are required for superconducting qubits and they need to interface with room-temperature optical data communications outside of the qubit refrigeration system. This work on stimulated emission rates versus temperature may prove invaluable for future high-speed quantum computing.

WAY AHEAD

Professor Feng's microcavity lasers have the potential to impact both long-range communications with remarkable improvements in error-free data rates and quantum information through cryogenic-to-ambient optical interfaces. In addition, small lasers of this nature are an important component of integrated optical computing concepts. If these advances are realized, it could revolutionize information processing

ARL Competencies:

- Photonics, Electronics, and Quantum Sciences
- Military Information Sciences
- Network Science and Computational Sciences

Results

- Led to sustained investment in developing a state-of-the-art optoelectronic characterization lab that enabled world-record, high-speed laser diodes poised for a new generation of optical communications links for distances from chip-scale to 2 km.
- Developed a small business program between ARO and DEVCOM C5ISR to pursue the cryogenic laser diodes to meet high-speed surveillance bandwidth demands of the future.
- Led to the cryogenic laser diode bandwidth increases enabled by this effort being pursued within IARPA "Supercables" for 4K quantum computing applications.

Anticipated Impact

Superior microlasers are expected to enable future leap-ahead technologies such as faster sensing and surveillance systems.

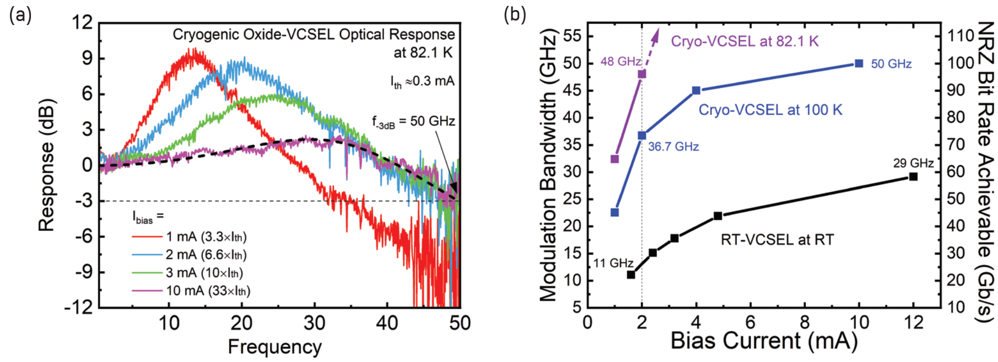


Figure 2: (A) The bias-dependent optical response of sdPhotonics' lasers at 82.1 K. (B) Performance comparison between the Cryo-VCSEL at 82 and 100 K, and the state-of-the-art 29-GHz RT-VCSEL. Adapted from Fu et al. (2020).

speeds. To further encourage discoveries, which can advance and bring these opportunities to reality for the Army, additional strategic investments are being made in high-speed, high-efficiency solid-state laser designs and the physical processes that emerge at higher frequencies.

SUCCESS STORY

Using Topological Physics to Overcome Integrated Photonic Circuit Challenges

ARO Presidential Early Career Award for Scientists and Engineers (PECASE) investment in novel topological physics approaches to optics resulted in two leading-edge publications in *Nature* poised to significantly transform integrated photonics.

CHALLENGE

The connection between optical elements in an optical system are a typical source of power loss and signal degradation. Planar lightwave circuits, aka photonic integrated circuits (PICs), have tremendous potential for military impact. Being extremely compact, they have the potential for revolutionizing the size, weight, power, and cost (SWaP-C) for Army applications. PICs can coherently combine laser light for directed energy and form extremely compact laser imaging detection and ranging (LiDAR) devices, extremely sensitive detectors for environmental sensing, and integrated platforms for information processing with revolutionary computing power. However, a couple of challenges prevent the realization of these concepts. PICs often incorporate bulky and power-hungry edge-emitting semiconductor lasers to illuminate photonic waveguides. External fiber illumination through the PIC surface is done by grating couplers. These couplers are known to have significant losses that hinder system efficiencies. Loss of light due to undesired absorption causes heating, degradation, and/or destruction of components and scattering of light, making the systems unsafe for power scaling. However, research based upon topological physics provides a new twist to photonic coupling and may overcome this previously untenable limitation, thus making possible many previously impossible applications.

There is a related challenge to the coupling of light into waveguides: the effectiveness of optical resonators at trapping light, which is important for lasers, filters, optical switches, and sensors. Materials and waveguides used within PICs naturally have variations, which prevent their development and ability to impact Warfighter capabilities. For example, the precision of placement and integrity of optical resonator features can be difficult to achieve because etching processes often create surface roughness and variations that scatter light or change the resonant frequency of the resonator. Photonic designs within waveguides to make them more tolerant to such variations could be game changing. Further, designs that minimize the effect of manufacturing errors on optical performance have the potential to improve the manufacturing yield of these nanophotonic devices.

ACTION

Dr. Gerhold began interacting with Dr. Bo Zhen of the University of Pennsylvania while he was still finishing his postdoctoral position at the Massachusetts Institute of Technology. Dr. Gerhold was impressed with Dr. Zhen's awareness of current scientific challenges related to integrated photonics, noting that Dr. Zhen had ongoing academic relationships with leading photonics institutes in Europe. Dr. Gerhold recognized that Dr. Zhen's credentials, impact, and vision would be competitive for a PECASE. Discussions between them led to Dr. Zhen submitting a proposal involving three thrusts to explore (1) "bound states in the continuum" physics for a unique type of nanophotonics resonances,

This success was made possible by:

Dr. Michael Gerhold,
Electronics Branch

Citations:

Jin, J. *et al. Nature* **574**, 501–504 (2019).

Yin, X., Jin, J., Soljačić, M., Peng, C. & Zhen, B. *Nature* **580**, 467–471 (2020).

"New Design Could Make Fiber Communications More Energy Efficient," *DEVCOM ARL Public Affairs*. (2020).

(2) ultrafast, low-energy switches based upon exceptional points, and (3) on-chip non-reciprocal devices based upon non-Hermitian modulations. This proposal was successful. Site visits and encouragement to pursue experimental verification of some nascent calculations led to significant publications early in the PECASE grant.

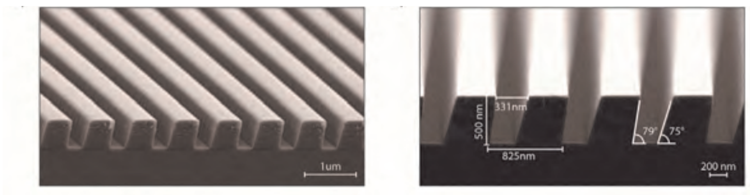


Figure 3: Scanning electron microscope images of actual fabricated optical couplers supporting unidirectional scattering. Adapted from Yin et al. (2020).

RESULT

Dr. Zhen was able to design and demonstrate a rather simple nanophotonic structure that scatters light only in one direction. These structures are a topological twist on an old concept: optical gratings. Physics ensures that gratings scatter light in multiple directions. A grating is simply a regular array of grooves in an optical material like glass. When the grooves are on the order of the light's wavelength, incoming light is redirected into two other directions, say, up and down. Dr. Zhen, however, recognized that the application of topological physics may be able to break this symmetry. By adjusting the angles at which the grooves were etched into an optical material, one of the scattering directions could be greatly reduced, if not completely eliminated. Using a new reactive ion etching method, he etched gratings at a slanted angle, with the outcome shown in Figure 3. The measured radiation asymmetry, defined as upward radiation divided by downward radiation, is presented in Figure 4. The highest measured asymmetry ratio is over 27 dB, meaning about 99.8% of the power radiates toward the top, reducing the downward radiation loss to only 0.2%. This is about 100 times better than commercial devices. That was with a fairly narrow wavelength band. Typical applications need to broaden the range of wavelengths that can be controlled. In this context, Dr. Zhen was able to demonstrate the redirection of 90% of light across a 26-nm-wide band to only one direction. In Figure 4b, he further shows that the device can cover a range of emission angles and is, thus, compatible with fiber arrays with different polishing angles commonly used in packaging. By providing a design that limits losses in grating-based couplers, this success will benefit a range of important DoD optoelectronic applications from quantum communications to LiDAR surveillance.

Dr. Zhen's PECASE-enabled work has also made inroads for enabling PICs to tolerate fabrication errors. In a photonic crystal (such as a grating or array of holes in an optical material), there are frequencies of light that get bound (localized, bouncing back and forth but unable to escape) inside the crystal simply because any light wave of a particular frequency that would escape interferes with another that cancels it out. Theoretically, this bound light would remain in the crystal indefinitely. In reality, there are limits due to crystal imperfections and the crystals are finite in size. Dr. Zhen exploited this concept and designed photonic crystals in which multiple bound states exist at a single specific frequency. In this case, the light becomes less sensitive to the influence of fabrication errors and poor surface finish, allowing the resonator to contain photonic signals for a longer time. Building on this insight, he designed, fabricated, and tested dozens of devices, which were intentionally "imperfect," with uneven surfaces visible under a scanning electron microscope. However, his unique design greatly improved the lifetime of the resonances: on average, he showed an enhancement over an order of magnitude (Jin et. al., 2019). This paves the way for increased manufacturing tolerances for photonic devices, which, in turn, paves the way for advanced optical technologies based on these design principles.

WAY AHEAD

Due to the Army relevance of these breakthroughs, Dr. Gerhold was selected by ARL leadership to highlight the potential of "Integrated Nanophotonics" for next-generation electronic and photonic systems at an Army Science Planning and Strategy Meeting in November 2020. Dr. Zhen's work is to be highlighted at this meeting. Dr. Zhen is also to lead a breakout roundtable discussion related to heterogeneous integration and optical coupling advances to provide the Army with concepts and strategies for advancing discoveries and developments advancing integrated nanophotonic technology.

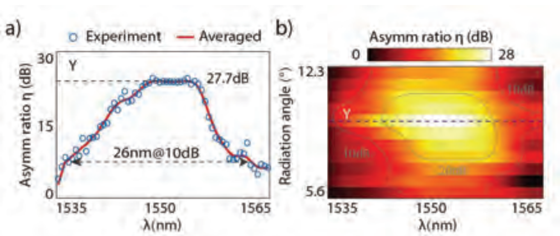


Figure 4: Experimental demonstration of unidirectional optical scattering. (A) A maximum directionality of over 99.8% is shown. (B) The coupling efficiency plot shows how the design works for a wide range of frequencies and fiber polishing angles. Adapted from Yin et al. (2020).

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Military Information Sciences

Network Science and Computational Sciences

Results

- Discovered, devised, and demonstrated photonic structures that preserve light two orders of magnitude better than state-of-the-art techniques, paving the way for the development of applications ranging from long-range surveillance, to communications, to optical information processing.
- Devised optical device designs that can reduce the effect of manufacturing variation across photonic crystals and improve the manufacturability of integrated photonic designs for lasers, detectors, and modulators both in classical and quantum optical circuits.

Anticipated Impact

This entirely new design approach is expected to enable future leap-ahead technologies such as higher-power and faster LiDAR and radar, and efficient information processing systems that exceed electronic counterparts by orders of magnitude.

SOLID-STATE ELECTRONICS AND ELECTROMAGNETICS PROGRAM

Program Manager
Dr. Joe Qiu

Dr. Qiu completed his undergraduate studies at the State University of New York at Stony Brook, receiving his B.S. in Physics in 1991. He trained as a physicist at the State University of New York at Stony Brook, receiving his Ph.D. in Physics in 1997.

He came to ARL in 2008 as an electronics engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.

Current Scientific Objectives

1 | Discover and create unique electromagnetic phenomena in solid-state materials and structures that require theoretical formulations beyond well-established Maxwell's equations that, if successful, will create new types microwave/millimeter-wave/terahertz devices that are electrically tunable.

2 | Create novel device concepts based on emerging phenomena in heterostructures and interfaces of engineered quantum materials that, if successful, will enable future electronic systems with significantly lower size, weight, and power and higher information process processing capacity.

3 | Develop novel electromagnetic structures to enable strong coupling with terahertz radiation (0.1-1 THz) and achieve efficient generation, manipulation, and detection of the aforementioned spectral range that, if successful, will potentially enable beyond-5G wireless communications in this part of the electromagnetic spectrum.

This success was made possible by:

Dr. Joe Qiu, Electronics Branch

Citations:

Qin, J.-K. *et al. Nat. Electron.* **3**, 141–147 (2020).

Wiles, K. “DNA-Like Material Could Bring Even Smaller Transistors,” *Purdue University News.* (2020).

SUCCESS STORY
Rare Earth Element Material Could Produce World's Smallest Transistors

Army-funded researchers at Purdue University have developed tiny transistors using single chains of atoms from a rare earth element, tellurium (Te). This breakthrough could produce world's smallest transistors and lead to smaller and faster computers.

CHALLENGE

Computer chips use billions of tiny switches, called transistors, to process information. The more transistors on a chip, the faster the computer. The famous Moore's Law originally stated that the density of transistors on a chip would double every year. Transistors on the market that are made of traditional bulkier silicon (Si) have shrunk from micrometers in size in the 1970s to 10-20 nm in scale. However, further decreases in the size of Si transistors has become challenging because of material limits. New materials and device design concepts are necessary to overcome these limitations and advance electronic computational technologies beyond the state of the art.

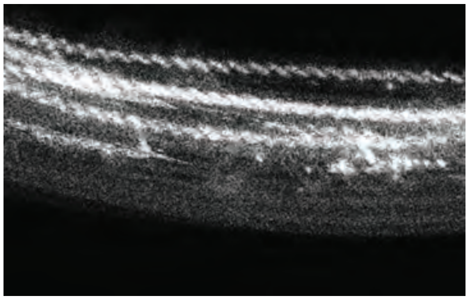


Figure 1: These silver, wiggling lines are strings of atoms in Te forming a helix like DNA. Researchers have not seen this behavior in any other semiconducting or metallic material. Adapted from Wiles (2020).

ACTION

The principal investigator for this project, Professor Peide Ye of Purdue University, was originally funded to work on 2D black phosphorous, a different type of new electronic materials. During the International Electron Devices Meeting in December 2017, he approached Dr. Qiu and told him that he had found an even more exciting material—Te, a van der Waals (vdW) material consisting of 1D helical chains instead of 2D sheets. He wanted to change direction

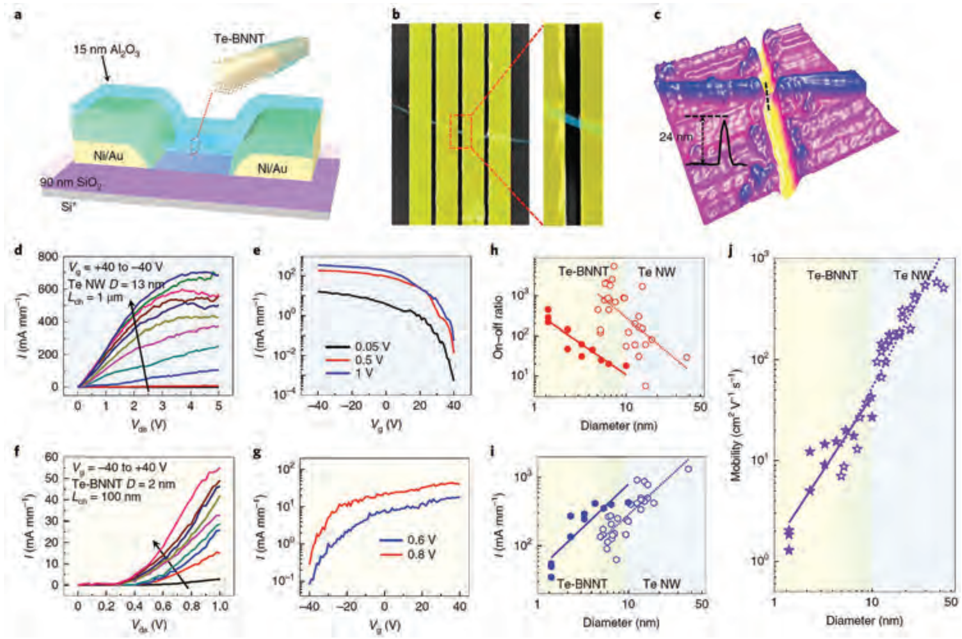


Figure 2: Electrical measurements of transistors based on few-chain Te NWs. (A) Schematic of an individual Te-BNNT FET. (B, C) False-colored scanning electron microscopy image and atomic force microscopy height profile of a representative FET device before alumina (Al_2O_3) capping. (D) Output characteristics of a typical p-type Te NW transistor with a diameter of ~13 nm. (E) Corresponding transfer curves of the same device. (F) Output characteristics of an n-type Te-BNNT transistor with a diameter of ~2 nm after 15-nm Al_2O_3 film capping. (G) Corresponding transfer curve, exhibiting typical n-type transport behavior with an on/off ratio of 450 at Vds = 0.6 V. (H) On/off ratio, (I) current density at Vds = 1 V, and (J) carrier mobility of Te-BNNTs and Te NWs short-channel FETs. Filled symbols represent Te-BNNT NW devices and open symbols represent bare Te NW devices. Adapted from Qin et al. (2020).

and work on this material instead. Dr. Qiu was initially skeptical, not sure if isolating a single atomic chain is possible. Despite the risk and given the opportunity for a potential breakthrough, Dr. Qiu encouraged Professor Ye to look for a solution to isolate a single atomic chain of Te. After two years of research, Professor Ye successfully developed an ingenious technique to achieve this.

RESULT

Over the past few years, transistors have been built as small as a few nanometers in lab settings. The ultimate goal is to build transistors the size of atoms. Professor Ye's lab at Purdue University is one of many research groups seeking to exploit materials much thinner than Si to achieve both smaller and higher-performing transistors. As reported in a Purdue University article in February 2020 (Wiles, 2020):

> *In 2018, the (…) team at Purdue discovered tellurene, a two-dimensional material derived from tellurium. They found that transistors made with this material could carry significantly more electrical current, making them more efficient.*
>
> *The discovery made them curious about what else tellurium could do for transistors. The element's ability to take the form of an ultrathin material in one dimension could help with downsizing transistors even further.*
>
> *One way to shrink field-effect transistors (FETs), the kind found in most electronic devices, is to build the gates that surround thinner nanowires.*

Professor Ye's group proceeded to elucidate the mechanisms required to isolate Te as a single atomic chain. Once accomplished, the group was able to build transistors with the chains. The 1D chains were compared to bare Te nanowires (NWs) synthesized by Professor Ye's colleague, Dr. Wenzhuo Wu of Purdue University, and collaborators at Washington University simulated the behavior of these thin NWs.

In a surprising "twist," the researchers discovered that these 1D chains are helical (Figure 1). The atoms strongly bond to each other in pairs to form DNA-like chains, which then stack through weak forces called vdW interactions to form a Te crystal (Wiles, 2020):

> *These van der Waals interactions would set apart tellurium as a more effective material for single atomic chains or one-dimensional nanowires compared with others because it's easier to fit into a nanotube.*

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Results

- Published in the prestigious journal *Nature Electronics*.
- Isolated, for the first time, a single 1D vdW atomic chain.
- Demonstrated the first transistor with a 1D vdW atomic chain.

Anticipated Impact

This research is expected to enable future computers and other electronic systems that are faster and consume less power.

Since the opening of a nanotube can't be any smaller than the size of an atom, tellurium helices of atoms could achieve smaller nanowires and, therefore, smaller transistors.

In a true testament to Professor Ye's collaborative spirit, his research group developed a transistor with a Te NW encapsulated in a boron nitride nanotube (BNNT) (Figure 2) that was provided by Professor Yoke Khin Yap of Michigan Technological University. The material's properties were characterized via Raman spectroscopy to benchmark its performance.

The excellent current-carrying capacity of Te atomic chains encapsulated in a boron nitride nanotube (Te-BNNT) strongly suggests that this nanomaterial system has potential for future electronics applications, especially high-performance FETs with ultrashort channels. The research was published in the journal *Nature Electronics* (Qin et al., 2020).

WAY AHEAD

The researchers will optimize the device to further improve its performance and demonstrate a highly efficient functional electronic circuit using these tiny transistors, potentially through collaboration with ARL researchers.

SUCCESS STORY

A New Ferroelectric van der Waals Heterojunction with Record-High Tunneling Electroresistance

Army-funded researcher at the University of Southern California has created a new type of memory device called ferroelectric tunneling junctions (FTJs) that demonstrate record performance utilizing atomically thin 2D vdW materials. This type of new structure can enable new memory devices with record performance in lowering energy consumption and reducing data corruption.

CHALLENGE

FTJ devices are part of a family known as nonvolatile memory devices, meaning they can be unplugged without losing their data. As the ferroelectric polarization field in these materials reverses direction, it can either facilitate the current flow (i.e., corresponding to an "on" setting) or block the current flow (i.e., corresponding to an "off" setting). These on and off settings can represent the "1" and "0" of digital information. FTJs need a very clear difference in states (i.e., to represent a "1" or "0"), which is controlled by what is termed the tunneling barrier. The tunneling barrier is described by the "height" that the energy needs to overcome in order to switch between states.

FTJs use a thin ferroelectric layer as a tunneling barrier, the height of which can be modified by switching its ferroelectric polarization. The junctions can offer low power consumption, nonvolatile switching, and nondestructive readout, and thus are promising for the development of memory and computing applications. However, achieving a high tunneling electroresistance (TER) in these devices remains challenging. Typical junctions, such as those based on barium titanate ($BaTiO_3$) or hafnium dioxide (HfO_2), are limited by their small barrier height modulation of around 0.1 eV.

ACTION

The principal investigator for this project, Professor Han Wang at the University of Southern California, is funded through ARO's Young Investigator Program (YIP; now Early Career Program [ECP]). Under the YIP award, which began in 2018, Professor Wang explored the use of emergent low-dimensional quantum materials for creating new electronic device concepts for memory and computing, which are highly relevant for future Army electronic systems. Professor Wang has a long history of working with ARL in-house researchers, starting when he was a graduate student at the Massachusetts Institute of Technology.

After Professor Wang started his tenure-track position, Dr. Qiu, together with Dr. Madan Dubey of ARL SEDD, visited him at the University of Southern California. During this trip, Dr. Qiu identified that low-dimensional transport is an area that is not well understood and could potentially enable many innovative device concepts with unprecedented performance. Furthermore, this research area offered many opportunities for collaboration between Dr. Wang, Dr. Dubey, and other ARL SEDD researchers because of mutual interest.

After the YIP award, Dr. Qiu encouraged Dr. Wang to continue his productive collaboration with ARL. As such, this ARO YIP award has allowed Dr. Wang to continue working with ARL, resulting in many high-quality joint publications with ARL researchers.

This success was made possible by:

Dr. Joe Qiu, Electronics Branch

Citations:

Wu, J. *et al. Nat. Elect.* **3**, 466-472 (2020).

"New Memory Device Extends Battery, Increases Upload Speed," *DEVCOM ARL Public Affairs.* (2020).

Paul, B. "Novel Technology Extends Battery Life, Increases Upload Speed, and Reduces Data Corruption," *USC Viterbi.* (2020).

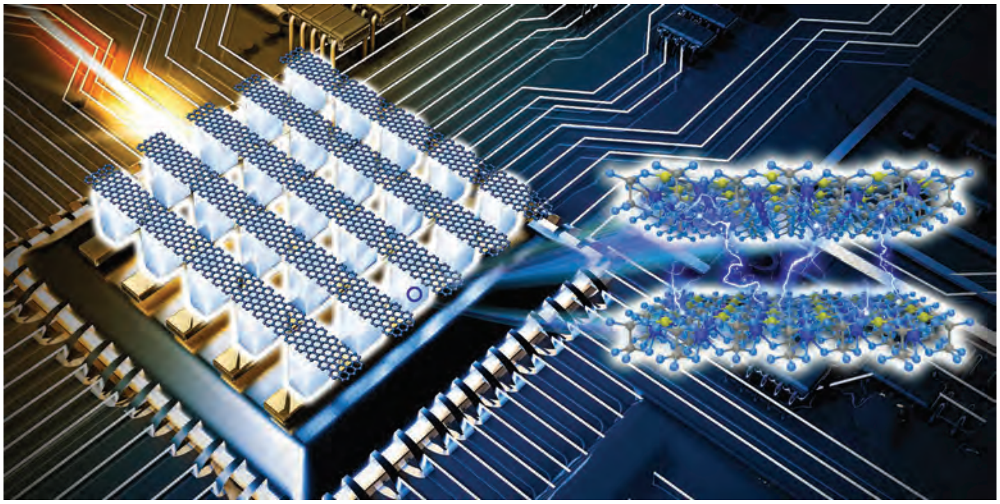


Figure 3: A schematic of the research team's new memory device. Adapted from Paul (2020).

RESULT

Traditionally, FTJ structures came in two primary forms: the most basic form utilizes metals as contacts on both sides of the junction, while a more recent structure replaces one of the metal contacts with a semiconductor material. The new device, utilizing asymmetric metal and semi-metallic graphene contacts, is able to exceed the performance of all previously demonstrated FTJs while offering promising prospects for integration with Si electronics. As reported by ARL's Public Affairs Office in July 2020:

> *More simply put, the unique properties of the new device, combined with a novel design structure, makes it much easier to distinguish between the different data states. And the better that can be done, the more reliably and efficiently data can be stored and processed. Furthermore, the unique advantage offered by van der Waals ferroelectric materials approaching atomic scale thickness can eventually lead to much faster and energy efficient ferroelectric tunneling junction memory.*

For the FTJ devices, Professor Wang used layered copper indium thiophosphate ($CuInP_2S_6$) as the ferroelectric barrier, and graphene and chromium as asymmetric contacts (Figure 3). The ferroelectric field effect in $CuInP_2S_6$ induced a barrier height modulation of 1 eV in the junction, which resulted in a TER of above 10^7 (Figure 4). This breakthrough was published in the prestigious journal Nature Electronics (Wu et al., 2020). In conclusion, the semimetal-ferroelectric vdW structure provides a new approach for achieving high giant barrier height modulation in FTJ devices, which is a critical step toward developing high-performance ferroelectric and multiferroic devices for memory and computing applications.

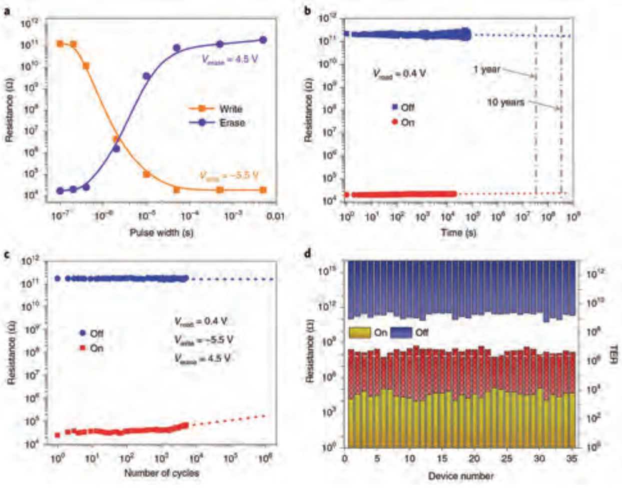


Figure 4: Performance of the vdW FTJ as a memory device: (A) Switch times of the FTJ from the off state to the on state and from the on state to the off state. (B) Data retention characteristics of the on and off states. (C) Endurance characteristic of the device. (D) Measured on- and off-state resistances and the TER for 35 FTJ devices. Adapted from Wu et al. (2020).

WAY AHEAD

Professor Wang and his fellow researchers hope that, with time, their device can be scaled up and may become a replacement not just for existing nonvolatile data storage, but also volatile memory, like D-RAM storage devices commonly found in computers. In addition, the device may also be engineered to hold multi-bit data states within a single cell, and with its robust endurance and retention, it has promising potential for applications in in-memory computing and other beyond-von-Neumann computing hardware.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Results

- Published in the prestigious journal *Nature Electronics*.
- Demonstrated record TER of 10^7, which is larger than any other FTJ devices.

Anticipated Impact

This new class of device has potential applications in energy-efficient computing hardware.

MATERIALS DESIGN PROGRAM

Program Manager
Dr. Evan Runnerstrom

Dr. Runnerstrom completed his undergraduate studies at Stanford University, receiving his B.S. in Materials Science and Engineering in 2009. He trained as a materials scientist at the University of California, Berkeley, receiving his Ph.D. in Materials Science and Engineering in 2016.

He came to ARO in 2019 as the Program Manager for the Materials Design Program.

Current Scientific Objectives

1. Generate new fundamental knowledge of self-assembly by elucidating the multiple physical and chemical forces at play during directed, bottom-up 3D assembly of super-structures that incorporate multiple components that, if successful, will support the deterministic design and creation of novel multi-functional materials, like biomimetic materials, with targeted properties, behavior, and capabilities.

2. Develop reconfigurable materials that can reversibly change their properties and hierarchically structured materials that display novel emergent or collective behavior that, if successful, will support the realization of advanced "smart materials" concepts like reconfigurable optics and electronics, dynamic signature management, and adaptive sensors.

3. Leverage recent advances in machine learning, artificial intelligence, data science, and other numerical approaches to solve difficult and complex materials design problems related to self-assembly and reconfigurability that, if successful, will enable data-driven, inverse design of advanced materials starting from desired properties and functionality, as well as novel models, algorithms, and experimental approaches to designing ever-more-complex materials.

This success was made possible by:

Dr. Evan Runnerstrom,
Materials Science Branch

Dr. John Prater (retired),
Materials Science Branch

Dr. Douglas Kiserow (retired),
Chemical Sciences Branch

Citations:

He, M. *et al.* *Nature* **585**, 524–529 (2020).

"Researchers Develop Method to Create Colloidal Diamonds" *NYU*. (2020).

SUCCESS STORY

Diamond and Beyond: New Horizons in Colloidal Self-Assembly

A decade of investment by ARO into the basic science underpinning colloidal particle self-assembly has resulted in fundamentally new capabilities for creating complex microscopic structures from the bottom up. These capabilities are poised to impact the Army's development of next-generation lasers and micro-robotics.

CHALLENGE

When thinking of optical materials, silicon solar panels or polycarbonate lenses in a pair of eyeglasses might come to mind. In these materials, atomic ordering dictates optical properties, but novel optical behaviors can also be achieved with larger-scale structures. Structural control of light at the nano- and microscale requires precise placement of microscopic particles into large periodic arrays. This is challenging because individual building blocks must be placed with nanometer-level precision, but periodic arrays must be tens of micrometers in size to interact with light effectively. Such structures are too complex to fabricate by top-down methods like lithography and thin-film deposition. Instead, a bottom-up, colloidal self-assembly approach is needed. Colloidal self-assembly utilizes liquid-suspended microscale particles that self-organize into a structure. This organization can be directed by physical forces, like gravity or entropy, or chemical directors, like engineered DNA sequences attached to the particle surfaces. Achieving the requisite control over colloidal assembly is challenging—one desires the assembly process to be responsive to external inputs like light or magnetic fields, and non-close-packed periodic structures like the diamond cubic lattice are very difficult to stabilize. Nonetheless, colloidal crystals assembled with diamond lattice symmetry (here, "diamond lattice" refers to the structural arrangement of the particles, not a gemstone) would represent an important step toward a long-standing goal in photonics: 3D photonic crystals with a photonic band gap (a range of frequencies where light cannot propagate) in the visible and infrared spectral range. Such photonic crystals would enable one to

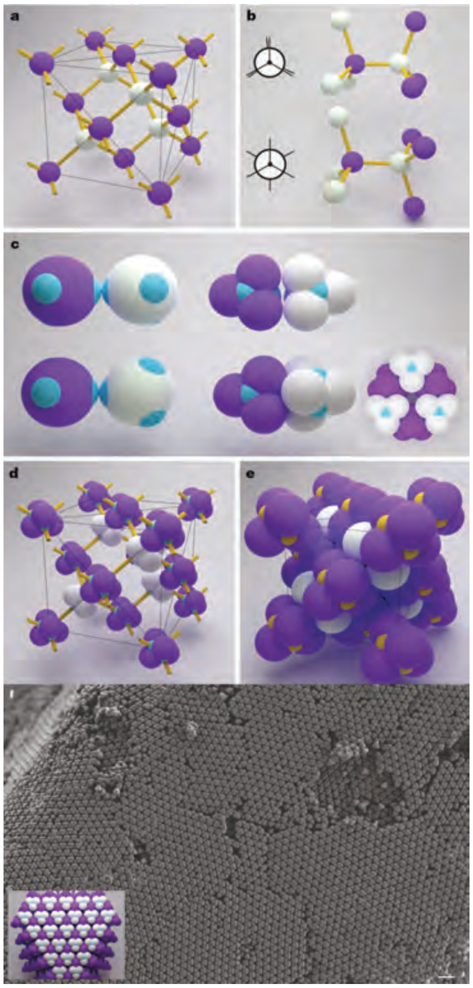


Figure 1: (A) Structural representation of the diamond cubic lattice. (B) The Newman projection with staggered tetrahedral bonding is a key building block that leads to diamond cubic symmetry. (C) Schematic representations of the interlocking self-assembly of tetrahedral colloids to form the diamond lattice. Spherical patchy particles are not forced to bind in a staggered geometry (left). Single-stranded DNA is attached to the core of each tetrahedron (highlighted in blue); when tetrahedra with complementary DNA strands (i.e., purple and white) encounter each other, the DNA binds them in the interlocking/staggered geometry (right). (D, E) Interlocking tetrahedral colloids build up the diamond lattice. (F) Scanning electron micrograph of self-assembled colloidal diamond crystals about 40 µm in size (scale bar 5 µm). Figure adapted from He et al. (2020).

control the flow of light with very precise waveguides, improve the design and performance of laser cavities, and control blackbody radiation for thermal signature management. Routes to create such a photonic crystal, however, have eluded researchers since the advent of photonic crystals in the late 1980s.

ACTION

The Materials Design Program Manager, Dr. John Prater (now retired), initiated a new programmatic research thrust focused on self-assembly and bottom-up materials science in the early 2010s. During this time, Dr. Prater organized colloquia through the Materials Research Society and developed a new Multidisciplinary University Research Initiative (MURI) topic (co-authored with Dr. Douglas Kiserow, now retired) titled "Directed Self-Assembly of Reconfigurable Materials." These actions established colloidal self-assembly and bottom-up materials science as strategic priorities for ARO.

The winning MURI proposal came from a team led by Professor Sharon Glotzer of the University of Michigan. The $7.5M project, "Reconfigurable Matter from Programmable Colloids," ran from 2010 to 2017 and brought together world-leading experts in soft matter theory, nanocrystal and colloidal particle synthesis and assembly, and hierarchical self-assembly. The stated goal of the MURI team, in response to the challenges laid out above, was to develop and deliver "the foundational knowledge and technical know-how to create an entirely new class of self-assembled, reconfigurable colloidal materials with radically increased complexity and functionality."

At the end of that MURI effort, Professor David Pine (New York University [NYU]) elegantly demonstrated that by carefully combining large spherical colloids with smaller tetrahedral colloid clusters, one could induce the assembly of a colloidal crystal by adopting a magnesium (Mg) and copper (Cu), $MgCu_2$, intermetallic structure. Coincidentally, the $MgCu_2$ structure is a combination of two interlaced diamond and pyrochlore lattices, both of which have robust photonic band gaps. This work was published in *Nature Materials* in 2017, and the result compelled Dr. Prater to invite a new Single Investigator (SI) proposal from Professor Pine to pursue self-assembled colloidal diamond and pyrochlore lattices.

The new project, "Self-Assembly of Colloidal Diamond and Related Lattices for 3D Photonic Band Gap Materials," began in 2017 and initially targeted the pyrochlore lattice. In early 2019, while trying to improve upon the $MgCu_2$/pyrochlore assembly methods, the researchers discovered that the tetrahedral building blocks (i.e., triangular pyramids), under certain geometrical conditions, would interlock in a staggered manner that supports the direct self-assembly of a diamond lattice. Using the Newman projection from organic chemistry as inspiration, the team realized that elemental diamond is the sole carbon allotrope consisting only of staggered tetrahedral bonds. The team switched their focus to this approach, carefully designing tetrahedral colloids consisting of four larger particles surrounding an interstitial core, which is functionalized with DNA strands. These DNA strands, combined with the proper tetrahedral geometry, force the particles to bind in a staggered conformation only. Ultimately, these designed colloids can only crystallize into a diamond lattice; other assemblies are not thermodynamically stable. Shortly after assuming his role as the new Program Manager for Materials Design, Dr. Runnerstrom conducted a site visit to NYU, where Professor Pine and co-workers briefed him on these new results. Realizing that a landmark result was in reach, Dr. Runnerstrom ensured that ARO would continue its support of the project.

ARL Competencies:

Sciences of Extreme Materials

Photonics, Electronics, and Quantum Sciences

Results

- Resulted in over 115 publications, 10 patent applications, 6 awarded patents, and publically available colloidal assembly simulation software.
- Led to Professors Glotzer and Pine being elected to National Academy of Sciences and the American Academy for Arts and Sciences, respectively.
- Demonstrated, for the first time, self-assembled colloidal diamond lattices, resulting in a *Nature* publication.

Anticipated Impact

Colloidal diamond lattices are expected to enable future leap-ahead technologies such as 3D photonic crystals for zero-threshold, high-efficiency lasers. Such lasers will be important for Army modernization in battlefield sensing and directed-energy capabilities.

RESULT

Professor Pine has perfected the method for creating self-assembled colloidal diamond, with the ability to create large colloidal crystals approaching 50 μm in size (Figure 1). This result, which is the first demonstration of reliable, scalable self-assembly of colloidal diamond, was published in *Nature* in September 2020 (He et al., 2020). This landmark publication represents the culmination not only of decades of work by Professor Pine and colleagues, but also over 10 years of work and investment by ARO's Materials Design Program.

WAY AHEAD

Dr. Runnerstrom worked with Professor Glotzer to secure a "Newton Award for Transformative Ideas during the COVID-19 Pandemic" through the DoD's Basic Research Office in summer 2020. Professor Glotzer's project, "A Microscopic Theory of Entropic Bonding," is laying a theoretical and data-driven foundation for understanding how the entropy associated with colloid shape can be used to rationally predict and design colloidal crystals. If successful, the results of this six-month project are expected to form the basis for a SI grant proposal under the "Computer-Aided Materials Design" thrust.

This success was made possible by:

Dr. Evan Runnerstrom, Materials Science Branch

Dr. Chakrapani Varanasi, Materials Science Branch

Dr. John Prater (retired), Materials Science Branch

Citations:

"Lasers Etch an Efficient Way to Address Global Water Crisis," *University of Rochester*. (2020).

Ranathunga, D. T. S., Shamir, A., Dai, X. & Nielsen, S. O. *Langmuir* **36**, 7383–7391 (2020).

Singh, S. C. *et al. Nat. Sustain.* **3**, 938–946 (2020).

Zhang, L., Guo, Z., Sarma, J. & Dai, X. *ACS Appl. Mater. Interfaces* **12**, 20084–20095 (2020).

SUCCESS STORY

Materials Surface Science for Water Purification

ARO basic research investment in chemical- and laser-based surface treatments has unveiled novel approaches for water purification. This may lead to new technology opportunities for providing clean drinking water to Warfighters in the field.

CHALLENGE

The Army and its Warfighters literally run on water—the availability and transport of freshwater is an enormous logistical challenge that pervades all aspects of operation, from sustainment, to expeditionary forces, to stabilization and humanitarian missions. To alleviate this burden, new methods are needed to harvest water at the point of need, either by capturing water vapor from the atmosphere or purifying contaminated water present in the environment. This is a formidable scientific challenge: the chemistry and physics of water and water vapor are such that it is very difficult to condense water vapor or remove contaminants—salt, heavy metals, and organic chemicals—without expending an inordinate amount of external fuel or energy (which would otherwise negate the logistical benefits).

ACTION

ARO Materials Design Program Managers Drs. Evan Runnerstrom, Chakrapani Varanasi (Acting), and John Prater (now retired) recognized that fundamental research into surface modifications and treatments was needed to better understand and tune how water molecules interact with a surface and with each other. In 2015, Dr. Prater awarded an SI grant, titled "Study of Functional Surface Structures on Metals," to Professor Chunlei Guo of the University of Rochester. The purpose of this project was to study how ultra-fast (femtosecond-length [fs]) laser pulses interact with highly reflective metals like aluminum to dramatically modify their surface structures. These modifications can render the metals to be highly light absorbing and significantly alters the liquid wetting properties of the surface. Over the course of the research, Professor Guo found that fs laser-patterned metals are super-hydrophobic (enough to even float on water) and also display super-wicking properties (i.e., the ability to draw water uphill against gravity with capillary forces).

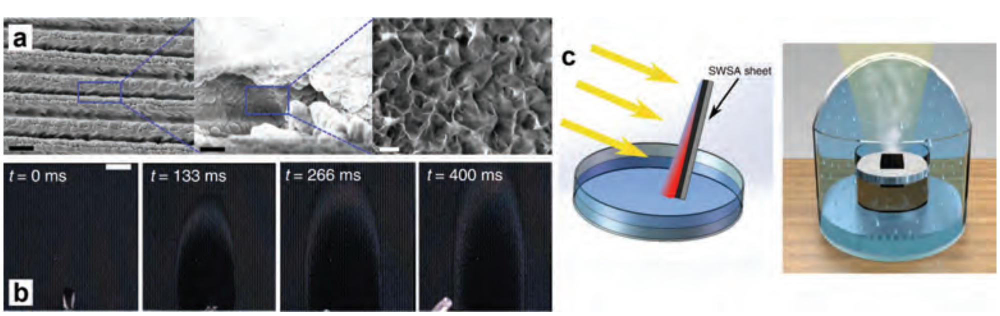


Figure 2: Laser-patterned aluminum panels for solar water purification. (A) Micrographs showing open capillary metal surfaces (scale bars left to right: 100 μm, 10 μm, 200 nm). (B) High-speed photographs of water super-wicking action. (C) Schematic illustrations depicting the solar distillation process. Figure adapted from Singh et al. (2020).

In 2019, Drs. Varanasi and Runnerstrom initiated a Young Investigator Program (YIP; now Early Career Program [ECP]) project with Professor Xianming "Simon" Dai of the University of Texas at Dallas (UT Dallas). The project, "Water Harvesting and Self-Cleaning on Air/liquid Independent Surfaces," aims to understand and control liquid-surface interactions in order to design and create patterned and chemically functionalized surfaces—"quasi liquid surfaces"—for passive water harvesting and decontamination. Professor Dai's unique approach is to investigate how fluids like water and oil interact with nanostructured surfaces, both with and without chemical functionalization, and the goal is to passively condense and remove water and other fluids from the surface. By combining nanostructuring and surface treatment, Professor Dai is exploring new routes to create durable and robust surface treatments that are long-lived, but display lubrication qualities similar to liquids. This approach will ideally offer good anti-fouling properties with long-term functionality, which is a persistent problem with existing technical approaches.

RESULT

Professor Guo leveraged the knowledge generated over the course of his research project to create a new aluminum panel that combines light absorption and super-wicking properties to act as a highly efficient solar water purifier (Figure 2). In July 2020, Professor Guo published results on such super-wicking and super-light-absorbing aluminum panels, and their ability to purify water, in *Nature Sustainability* (Singh et al., 2020). By using fs lasers to create hundreds of microscopic trenches on aluminum surfaces ("open capillaries"), with structured nanoscale roughness within the capillaries, the aluminum was made simultaneously super-wicking and highly light absorbing. The absorbed light quickly transforms into heat, which is immediately conducted into the water within the capillaries, very quickly evaporating the water to allow efficient, solar-based water distillation and purification. The combined super-wicking and super-light-absorbing properties of the aluminum panel provided exceptional water purification performance, even outperforming a theoretical device that perfectly converts solar energy into heated water (Professor Guo hypothesized that the open capillaries reduced the overall energy required to evaporate water). The panel was able to generate up to 1.26 L of water per hour (per square meter of panel) and also reduce chemical contamination below World Health Organization standards for safe drinking water.

In April 2020, Professor Dai published "Passive Removal of Highly Wetting Liquids and Ice on Quasi-Liquid Surfaces" in *ACS Applied Materials and Interfaces* (Zhang et al., 2020). Professor Dai used polydimethylsiloxane to form brushes that retained the flexibility commonly associated with silicone. This chain mobility and the grafting process results in a robust coating that is very hydrophobic, allowing water to slide across the surface. These surfaces exhibit durable fog harvesting over 4+ h without losing their hydrophobicity or surface lubrication properties, outperforming the harvesting and durability performance of other state-of-the-art coatings. Professor Dai and colleagues at UT Dallas followed up with simulation studies (Ranathunga et al., 2020), shedding new light on how water condenses onto these surfaces, providing new insight on how to tune this wettability behavior to maximize water harvesting.

WAY AHEAD

Professor Guo will work to optimize the water purification performance of the aluminum panels. Because the open capillary structures are easily cleanable and because aluminum is lightweight, initial results suggest this technology could be adapted for water purification in the field—a 3.5 ft x 1 ft sheet of aluminum could potentially generate a day's worth of drinking water for a Soldier given 12 h of sunlight.

Dr. Runnerstrom is working with DEVCOM SC researchers focused on Soldier-level water purification to identify potential transition and technology development opportunities based on both Professor Guo's and Professor Dai's work. Dr. Runnerstrom is also leveraging water-related scientific activity in the Materials Design Program to provide technical support to a new Defense Advanced Research Projects Agency (DARPA) program, Atmospheric Water Extraction (AWE) (Program Manager: Dr. Seth Cohen), as a subject-matter expert for proposal reviews. As the AWE program kicked off in late 2020, Dr. Runnerstrom was selected to serve as a Contracting Officer's Representative in order to provide continued technical support for the program for the next several years.

ARL Competencies:

- Sciences of Extreme Materials
- Photonics, Electronics, and Quantum Sciences
- Biological and Biotechnology Sciences

Results

- Published in *Nature Sustainability* describing exceptional solar water purification performance from aluminum panels.
- Initiated a new ECP project to develop robust surface treatments capable of harvesting water from fog, with two publications and one patent application.
- Led to the ARO Program Manager now supporting a new DARPA program in AWE—results from this ARO program may prove useful for DARPA's technology development.

Anticipated Impact

Laser-based and polymer-based materials surface treatments are expected to enable future leap-ahead technologies for harvesting and/or purifying drinking water at the point of need.

MECHANICAL BEHAVIOR OF MATERIALS PROGRAM

Program Manager
Dr. Daniel Cole

Dr. Cole completed his undergraduate studies at the State University of New York at Geneseo, receiving his B.A. in Physics in 2004. He trained as a mechanical engineer at the University of Maryland, receiving his Ph.D. in Mechanical Engineering and Materials Science in 2009.

He came to ARO in 2019 as the Program Manager for the Mechanical Behavior of Materials Program.

Current Scientific Objectives

1 | Discover material phenomena that enable extreme mechanical behaviors through dramatic improvements in energy dissipation, toughness, stiffness, hardness, and resiliency, to include new understanding, control, or confinement of deformation mechanisms; exploiting heterogeneous material systems and interface/interphase interactions to enable unprecedented properties while avoiding inherent sub-system weaknesses; and novel approaches for materials to perform in extreme thermomechanical environments, that, if successful, would enable new technologies for Soldier and vehicle protection, advanced propulsion systems, and hypersonic applications.

2 | Investigate structural materials that actively respond to dynamic loading environments and other external stimuli through rapid adaptation of shape, topology, or mechanical properties, to include mitigation or manipulation of stress wave propagation; novel actuation schemes that generate extraordinary forces or require minimal input energies; and novel material responses initiated through multiaxial loading, that, if successful, would enable unprecedented capabilities for protection, maneuver, and reconfigurable systems.

This success was made possible by:

Dr. Daniel Cole, Materials Science Branch

Dr. David Stepp, ARO Chief Scientist

Dr. Julia Barzyk, Mechanical Sciences Branch

Citations:

Kozlowski, R. *et al. Phys. Rev. E* **100**, (2019).

SUCCESS STORY
Stick-Slip Dynamics in Granular Materials

This effort has helped the Army understand the mechanical behavior of systems of rigid particles, providing important insight into deformation and damage mechanisms in materials, including phenomena preceding failure events. This work is expected to inform the failure dynamics of hard armor systems and potentially lead to technologies for resisting or steering damage progression in future protective materials.

CHALLENGE

The ability to predict how materials deform and fail is important for a number of Army applications, including armor, penetrators, vehicle structures, and reconfigurable autonomous systems. Many solid materials can display fluid-like behaviors as they deform. The study of granular media has been identified as a test bed for understanding fundamental mechanisms of solid-fluid behaviors. While the behaviors of granular systems had long been studied in the geological sciences community, there were significant gaps in the fundamental understanding of the failure mechanisms and the ability to predict precursors to failure events. The complexity of these systems and the associated behaviors have long limited progress in these areas. One example is identifying the controlling multiscale mechanisms of stick-slip behaviors: what are the key features of the granular systems that precede and accompany slip failures, how does particle shape affect the stick-slip dynamics, and how does particle friction affect the behaviors?

ACTION

Solid-fluid behaviors of materials had long been a priority for the Mechanical Behavior of Materials Program. In 2011, Dr. David Stepp, former Program Manager, looked into the phenomenon of shear jamming in soft condensed matter. The program supported a 2011 Gordon Research Conference that highlighted a range of new developments related to soft matter far from equilibrium and included discussions on shear jamming (the point at which a liquid suspension becomes solid-like via shear

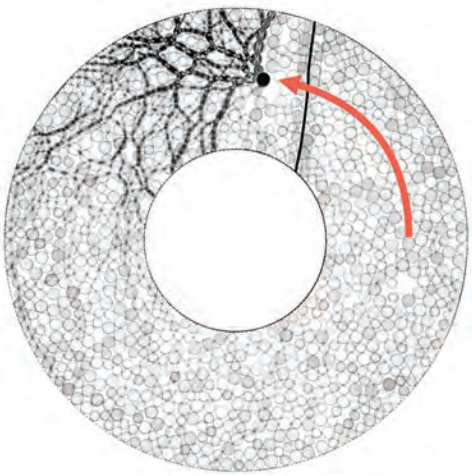


Figure 1: Photoelastic image shows stress accommodation through force chains in a granular system made up of rigid 2D discs. The arrow indicates the movement of an "intruder" grain that is driven through the granular media at constant angular velocity. Figure adapted from Kozlowski et al. (2019).

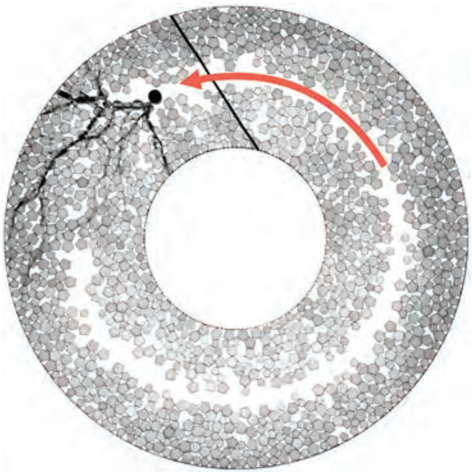


Figure 2: Photoelastic image shows stress accommodation through force chains in a granular system made up of rigid 2D pentagons. Note that the force chains in the 2D pentagon system appear sparser and straighter with respect to the 2D discs (shown in Figure 1). Figure adapted from Kozlowski et al. (2019).

loading). In 2012, Dr. Stepp partnered with Dr. Samuel Stanton, Program Manager of the ARO Complex Dynamics and Systems Program, to fund a research project exploring the jamming/unjamming transition in particle-based systems. Given the progress made in understanding jamming behaviors in soft condensed matter, and partially motivated by the need in the ceramic armor community for fundamental understanding of rigid granular flow, Dr. Stepp began exploring similar phenomena in hard particle systems.

In collaboration with DEVCOM SC and ARL, a Small Business Technology Transfer (STTR) project run through the Mechanical Behavior of Materials Program highlighted this need. The STTR effort, led by Transparent Armor Solutions and Southwest Research Institute, investigated the multi-hit performance of small-arms protective armor. During impact events, the ceramic materials can fracture and result in a spider-web-like pattern of material. These impacts and subsequent impacts resemble the flow of granular media. The STTR effort attempted to predict the material response when subsequent events occur at various positions relative to an initial event.

Previous investigations into the collective behavior of rigid particles had identified force chain networks that develop within the system to carry the load. A team led by Dr. Joshua Socolar at Duke University proposed investigating the fundamental mechanisms of these systems upon application of force, with the goal of understanding the conditions preceding large stick-slip events. Recognizing the opportunity to greatly enhance the understanding of these hard granular flow issues, Dr. Stepp selected Dr. Socolar's effort for a Single Investigator award in 2018.

RESULT

Dr. Socolar's group initially focused on 2D experiments using photoelastic methods (i.e., techniques that measure variations in the optical properties of a material through mechanical deformation). These methods were used to characterize the internal stresses of a particle system in response to an "intruder." The intruder consisted of a rod with a diameter approximately the size of a grain and was driven by a motor moving at constant speed. As the local stresses increased in and around the rod, force chains developed in the system and carried the imposed loads in non-trivial ways (Figure 1). As the yield stress of the given jammed configuration was exceeded, the intruder slipped forward until a subsequent jammed configuration was observed. The team attempted to understand how the particle properties (e.g., size, shape) influenced the dynamics of the flow.

A detailed look at the disc grain system showed that the flow behavior was dominated by two dynamic regimes. The first was intermittent flow, where the intruder moved relatively freely but occasionally became stuck. The second regime was dominated by a series of stick-slip dynamic events in which the intruder advanced via a sequence of distinct and rapid movements. The team also performed a series of simulations that largely agreed with the experimental results. The simulations were used to explore a broad range of the parameter space and inform future experiments. The frictional behaviors of the particle system were a focus of the modeling efforts, since these parameters were difficult to vary smoothly through experiments. The group has also explored the stick-slip behaviors of systems of particles with more complicated geometries. For example, Figure 2 displays a photoelastic image of a system of

ARL Competencies:

- Sciences of Extreme Materials
- Terminal Effects
- Mechanical Sciences

Results

- Demonstrated the theoretical calculations and experiments that govern the mechanisms of stick-slip behaviors in granular systems.
- Transitioned, through journal publications and internal progress reports, to several ARL in-house scientists investigating failure mechanisms in hard armor.

Anticipated Impact

Understanding the physics of granular flow is expected to enable future leap-ahead technologies for damage-adaptive protection systems for the Soldier.

pentagon-shaped particles subject to an intruder. From the preliminary experiments on the pentagon system, the force chain networks appear sparser and straighter with respect to the system of discs.

Fundamental studies of stick-slip behavior in granular systems are expected to assist Army engineers to develop advanced computational design tools for future armor systems. If the researchers are able to understand the conditions in which a large granular stick-slip event occurs, this could potentially help engineers design protection materials that could manipulate the fracture behavior and possibly steer loads away from vulnerable areas.

WAY AHEAD

In the last year of this effort, the team is focusing on the stick-slip dynamic behaviors in 3D systems of grains. One of the main goals of these future efforts is to develop methods for detecting precursors to large stick-slip events. If successful, this work could provide a foundation for understanding how complex failures occur in materials and potentially how these mechanisms could be manipulated to promote damage-tolerant and healing behaviors for future Army systems. In particular, the work is expected to augment work like the STTR project investigating the multi-hit performance of small-arms protective gear, along with similar applied research efforts ongoing in ARL WMRD.

This success was made possible by:

Dr. Daniel Cole, Materials Science Branch

Dr. David Stepp, Chief Scientist

Citations:

Hsieh, S. *et al. Science* **366**, 1349-1354 (2019).

SUCCESS STORY

High-Pressure Mechanochemistry

This investigation established methods for determining the response of materials in extreme pressure and shear environments, which are expected to enable new understanding of armor and may also enable new strategies for processing superhard materials.

CHALLENGE

Many Army materials are expected to perform in extreme mechanical environments. Materials may be designed to accommodate high-strain-rate events, withstand great thermomechanical loads, endure high cyclic loading, or sustain intense vibrations over a wide frequency range. These extreme environments can alter the mechanical, chemical, and electrical properties of materials. However, these extreme conditions are often difficult to reproduce in a controlled laboratory setting. The ability to carefully interrogate the material in the loaded condition can reveal important information about the mechanochemistry (i.e., the coupling of chemical and mechanical phenomena). In particular, ceramic materials are challenging to study, since the pressures required to study these phenomena are typically in the gigapascal region. However, these loading conditions are in the range in which armor materials are expected to perform, so these studies are of great interest to Army scientists.

ACTION

Dr. Valery Levitas of Iowa State University had originally been awarded a grant monitored by the ARO Synthesis and Processing of Materials Program several years ago focused on developing tools for measuring the high-pressure response of ceramics. Recognizing the experimental capabilities developed in this initial project, Dr. David Stepp, former Program Manager of the Mechanical Behavior of Materials Program, awarded an effort to investigate the high-pressure and high-shear behavior of ceramics with a focus on understanding the phenomena that could enable enhanced energy absorption in these extreme environments. Dr. Stepp continued the active engagement throughout the life of this project, at one point supporting an instrumentation project for a high-pressure and high-shear cell that could be integrated into a synchrotron system for in situ x-ray diffraction studies. This led to successful collaborations with Department of Energy scientists. In the final year of this project, Dr. Cole worked with key ARL researchers to arrange an invited talk for Dr. Levitas at Aberdeen Proving Ground, Maryland, in 2020. Dr. Levitas presented an overview of the ARO-sponsored work, toured facilities, and held discussions with several Army scientists to discuss potential opportunities to collaborate.

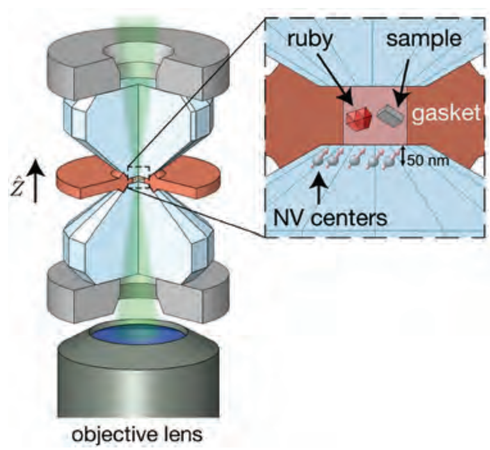


Figure 3: Schematic of high-pressure cell design allowing for material characterization at various spatial locations, which is critical for determining pressure-dependent yield strength, friction conditions, as well as phase transformation criteria. Figure adapted from Hsieh et al. (2019).

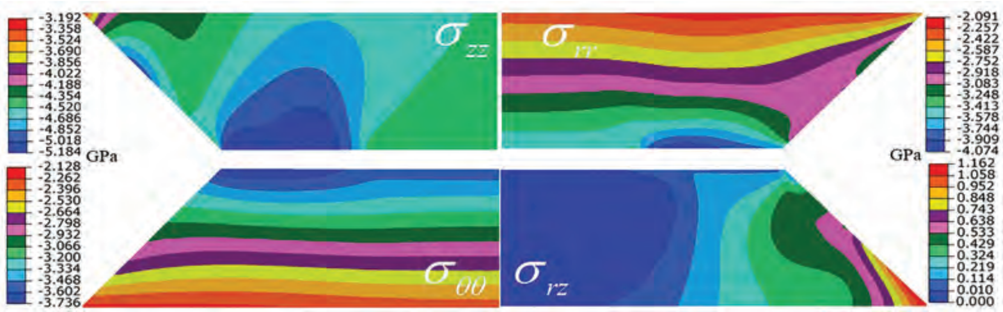


Figure 4: Model of the stress fields within the high-pressure cell. These simulations helped to optimize the pressure cell geometry to obtain the maximum loading conditions, as well as inform the mechanophysical processes that occur at different spatial locations within the sample. Adapted from Hsieh et al. (2019).

RESULT

Many previous ceramic mechanochemistry investigations have focused on studying the response of materials in a high-pressure cell, often through optical spectroscopy techniques. A great challenge for these experiments was the inability for researchers to measure how the mechanical loading varies spatially throughout the material. The extreme stress gradients generated around the sample limit most spectroscopy techniques. Thus, researchers would typically measure the bulk properties averaged over the entire cell geometry. Additionally, most existing loading cells were only capable of imparting uniform pressure on samples. Combinations of high pressure and shear stress (i.e., stress parallel to the loaded surface) were much more difficult to impose, yet these combined stresses are often more realistic for Army materials operating in extreme environments.

Dr. Levitas helped pioneer development of an instrument known as a rotational diamond anvil cell (RDAC). The setup consists of two diamonds compressing a sample, with one of the diamonds capable of simultaneously rotating and creating a combined pressure and shear environment. The team integrated the RDAC into a synchrotron for x-ray diffraction characterization to reveal information about in situ phase transformations under compression and torsion. The instrument was used to measure the radial distribution of stress within various ceramic materials. What the team discovered was that the pressures in the different phases of material could vary significantly. Simulations revealed that plastic shear strain could act as a substitute for thermally activated nucleation of the high-pressure phase. This discovery was significant because it showed how this combined pressure and shear loading could induce phase transformations non-uniformly, which could be both detrimental (e.g., lead to premature failures of structural materials) or potentially beneficial (e.g., inform new approaches to synthesizing advanced structural materials).

To provide additional fidelity with these high-pressure experiments, the group partnered with researchers at University of California, Berkeley and the Lawrence Berkeley National Laboratory to develop a loading cell with a layer of nitrogen vacancies at the diamond surface (labeled NV centers in Figure 3). The nitrogen vacancies were sensitive to local changes in mechanical loading and were used to determine the stress fields at the boundary of the sample, which enabled the recreation of the stress tensor over the entire diamond anvil through simulation (Figure 4). These results enabled new ways to determine the fracture criteria of diamond and allowed for the optimization of the cell geometry to reach the maximum possible pressure. The results of this study were highlighted in a 2019 *Science* paper (Hsieh et al., 2019).

Interestingly, the team also used these high-pressure and high-shear environments to create new materials. The RDAC was used to discover a new shear-induced phase of boron nitride that was extremely hard and even scratched the diamond cell. The group also demonstrated a new technique for converting graphite into diamond. Graphite, which is known to transform into diamond at approximately 70 GPa of hydrostatic pressure, was transformed into the diamond phase within the RDAC at 0.7 GPa of pressure when combined with moderate plastic shear. The ability to reduce the applied pressure to obtain diamond from graphite by approximately 100 times less than the known hydrostatic process could enable new strategies for low-pressure, shear-induced synthesis.

WAY AHEAD

This investigation has developed new tools to characterize and simulate material response under high-pressure and high-shear environments, which is a crucial foundation for researchers to understand how armor responds to impact events. In addition, this work could potentially inform Army investigations on materials for armor-piercing munitions, given that new insights on how advanced ceramic materials respond in extreme environments could enable new technologies for defeating hard armor. The tools created in these studies could potentially be used to evaluate candidate protection and lethality materials that may be of interest for advanced Soldier protection and the Next Generation Combat Vehicle.

ARL Competencies:

Sciences of Extreme Materials

Terminal Effects

Results

- Developed experimental techniques and simulations for studying combined high-pressure and high-shear environments.
- Led to co-publications between an ARO-funded researcher and Department of Energy scientists.
- The principal investigator delivered an invited seminar at ARL in 2020.

Anticipated Impact

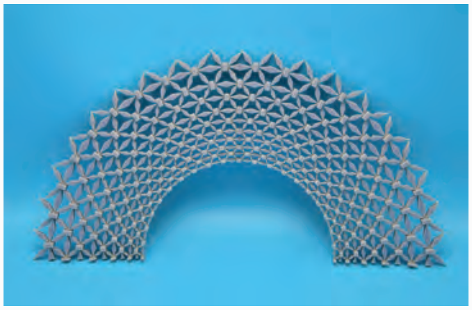
Understanding the phase transformation behavior of ceramics under extreme mechanical environments is expected to enable future leap-ahead technologies for creating and predicting the performance of advanced armor for Soldier and vehicle protection.

Designing a flexible material to protect buildings, military personnel

MU engineers said their material has both civilian and military applications

MIZZOU NEWS, UNIVERSITY OF MISSOURI | MAY 26, 2020

A team of engineers at the University of Missouri has designed a flexible material that can help buildings withstand multiple waves of energy traveling through a solid material, including the ground motions found in earthquakes.



Even though they are miles from the epicenter of an earthquake, buildings can collapse due to how an earthquake's energy makes the ground shake and rattle. Now, a team of engineers led by Guoliang Huang, a James C. Dowell Professor in the Mechanical and Aerospace Engineering Department at the University of Missouri College of Engineering, has designed a flexible material that can help buildings withstand multiple waves of energy traveling through a solid material, including the simultaneous forward and backward and side-to-side motions found in earthquakes.

"Our elastic material can stretch and form to a particular surface, similarly to a wrap on a vehicle," Huang said. "It can be applied to the surface of an existing building to allow it to flex in an earthquake. What is unique about the structured lattice-type material is that it protects against both types of energy waves — longitudinal and sheer — that can travel through the ground." Huang said the material also can be used by the defense industry to protect against vibration in mechanical parts, such as aircraft or submarine engines.

"For over 20 years, no one had a natural solution for this issue in a solid material," Huang said. "Now, we've designed, modeled and fabricated a new material with properties that do not exist naturally for what we believe is a nearly perfect protective device."

The Army Research Office, which provided funding for the basic research effort at the University of Missouri associated with this project, is encouraged by the results from Huang's team. "The results that the University of Missouri team has recently published are encouraging," said Dan Cole, the program manager at the Army Research Office, a part of the U.S. Army Combat Capabilities Development Command's Army Research Laboratory. "This research could lead to new strategies for steering mechanical waves away from critical regions in solid objects, which could enable novel capabilities in soldier protection and maneuvering."

The studies, "Polar Metamaterials: A New Outlook on Resonance for Cloaking Applications" and "Physical Realization of Elastic Cloaking with a Polar Material," were published in Physical Review Letters, a journal of the American Physical Society.

Chief Scientist Spotlight | Dr. David M. Stepp
Chief Scientist, ARO

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his bachelor's degree in Engineering in 1993. He studied Mechanical Engineering and Materials Science at Duke University, receiving his Ph.D. in 1998.

He came to ARO in 1999 as the Program Manager for the Mechanical Behavior of Materials Program. He became the Chief of the ARO Materials Science Branch (formerly Division) in 2004, the Director of Engineering Sciences in 2016, and the ARO Chief Scientist in 2020.

Structural materials are inherently susceptible to damage. Given the complex and intense types of damage that occur on the battlefield, materials designed to protect personnel and materiel have long been considered passive in function, and have thereby been designed and enhanced with strength and mass to resist deformation. New scientific discoveries supported by ARO in the mid-2000s identified an emerging opportunity in the area of productive mechanochemistry, where forces induced by mechanical stress could be harnessed and used to drive predefined, beneficial chemical reactions. Specifically, sensing an opportunity for a disruptive breakthrough, ARO Mechanical Behavior of Materials Program Manager, Dr. Stepp, and former Polymer Chemistry Program Manager, Dr. Douglas Kiserow, organized a unique workshop in January 2006 to bring internationally renowned researchers in the areas of self-healing and self-repairing polymers and materials together with DoD scientists and engineers to establish emerging research opportunities.

This workshop identified a particular opportunity in the area of productive mechanochemistry with research targets such as new compositions of matter, mechanochemical transduction, molecular reconfiguration before failure, and advances in reversible chemistry. Later that same year, Drs. Stepp and Kiserow devised the first-ever multidisciplinary research opportunity at the forefront of materials and mechanochemistry, calling for "molecular dynamic and thermodynamic theory to be extended to describe mechanochemical transduction, to develop predictive computational methodologies, and to guide the rapid design and synthesis of novel mechanophores." This opportunity not only defined the etymology of "mechanophore" (a force-activated molecular unit), but captured the imagination and attention of researchers internationally who envisioned the ability to embed these force-activated molecules into polymeric materials to realize a range of new materials with Army-relevant functional capabilities such as early-warning indicators for failure and the ability to remodel and strengthen in response to mechanical stress. Furthermore, these results identified a new possibility of tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress waves and control energy dissipation. The materials science and chemistry research communities established new frontiers of science in force-activated materials that could respond directly to an applied force to provide useful functions and drive chemical reactions; however, the overlap with protective materials remained out of reach due to the intense stresses and levels of protection required.

In 2015, building off significant progress in mechanochemistry and the new opportunities this work was generating in related scientific disciplines, Dr. Stepp invited a unique proposal to explore and predict theoretical cloaking in elastodynamics. Building off the success demonstrated with novel molecules synthesized for mechanochemistry, interest was growing in other ways that materials could be designed to respond to the application of forces and respond to those forces directly. The design of metamaterials that could achieve a limited degree of optical cloaking provided additional inspiration for a mechanical analogue. Elastodynamics is the study of elastic waves (i.e., small and reversible mechanical or stress waves in solid materials) with variation in time. Furthermore, cloaking in elastodynamics would provide the ability to isolate (i.e., shield or cloak) regions of a material or structure from stress waves. This constituted a highly disruptive scientific opportunity with exceptional relevance for the Army. In particular, materials that could localize all the applied deformation energy to an isolated region of the material, or "steer" or otherwise manipulate stress waves and deformation energy in material would provide revolutionary advances in protective materials, including personnel protection, vehicle armor, and extremely resilient structural materials. Professor Arash Yavari at the Georgia Institute of Technology, with ARO support, developed, for the first time, a mathematically precise formulation of elastodynamic cloaking to enable design guidelines for hiding cavities from elastic waves. This theoretical work elucidated the challenges associated with the experimental realization of elastodynamic cloaking, and identified a particular need for a highly tunable processing strategy to fabricate precise materials that could be embedded with the features necessary to manipulate (and ultimately cloak) applied stresses.

In 2017, motivated by the groundbreaking work of Professor Yavari and eager to identify scientific breakthroughs to overcome these challenges, ARO provided support for an extremely promising research proposal from Professor Guoliang Huang at the University of Missouri. That work, which produced this press release in 2020, identified a new paradigm for protective materials by overcoming the longstanding challenges that have prevented the discovery of materials capable of mitigating the propagation of deformation stress waves and even energy dissipation. The key breakthrough underlying this result is a rotationally resonant metamaterial based on torque-induced, non-symmetric stress states and collapse mechanisms. Rotating resonators precisely designed into the material can exert a density of torques that can interfere with and even mitigate (or "cloak") pressure and shear waves applied to the material. While these results do not yet approach the intensity and complexity of pressure and shear waves that occur regularly on the battlefield, they constitute an extraordinary new paradigm for "active" protective materials with unique features and artifacts to provide significant additional protection and resistance to damage and deformation.

Both the theoretical and experimental portions of this work have been shared and discussed extensively with in-house protection materials and extreme materials experts within ARL. Potential long-term applications include functionally graded cloaking devices that can guide elastic waves from explosions or impact loads away from a critical structure (e.g., to maintain a building's integrity after ballistic impact or earthquakes) or the Soldier (e.g., to reduce the incidence of traumatic brain injury by deflecting blast energy away from the brain).

The efforts described here are great examples of the type of interactions that lay the foundation for ARO's mission "to create and direct scientific discoveries for revolutionary new Army capabilities." Without the recognition by ARO Program Managers that the challenges inherent to materials science could be mitigated by advances in polymer chemistry, these two fields may have worked in silos, curtailing the rate of discovery for this cross-discipline capability. By advocating for novel material properties, embracing the synthesis of new materials, and developing the theory to predict materials that do not yet exist, scientific discovery is further enhanced.

PHYSICAL PROPERTIES OF MATERIALS PROGRAM

Program Manager
Dr. Chakrapani (Pani) Varanasi
Chief (Acting), Engineering Sciences Division

Dr. Varanasi completed his M.S. in Materials Science and Engineering at the Indian Institute of Technology, Kanpur, India in 1990. He trained as a materials scientist at the University of Notre Dame, receiving his Ph.D. in Materials Science & Engineering in 1994.

He came to ARO in 2009 as the Program Manager for the Physical Properties of Materials Program and was promoted to Branch Chief, Materials Science Branch in 2017.

Current Scientific Objectives

1 | Discover materials of novel compositions and structures with extraordinary physical properties (electronic, photonic, magnetic, and thermal) through a fundamental understanding of nucleation/growth mechanisms, reaction kinetics, interface control, and composition/structure control during top-down approaches that, if successful, will impact the Army's transformational overmatch capabilities in the areas of sensing, communication, power, and energy.

2 | Develop extraordinary characterization techniques using the latest technological developments to explore functional properties of novel materials as well as develop an understanding of the influence of defects in materials on the functional properties to establish defect-property correlations that, if successful, will play an important role in transforming applications in sensing, communication, power, and energy.

This success was made possible by:

Dr. Chakrapani Varanasi,
Materials Science Branch

Dr. Dawanne Poree,
Chemical Sciences Branch

Citations:

Day, R. *et al. ACS Cent. Sci.* **5**, 1959–1964 (2019).

Dou, J.-H. *et al. Nat. Mater.* (2020).

Feriante, C. *et al. J. Am. Chem. Soc.* **142**, 18637–18644 (2020).

Skorupskii, G. *et al. Nat. Chem.* **12**, 131–136 (2020).

SUCCESS STORY
Novel Organic Materials with Extraordinary Functional Properties: Two-Dimensional van der Waals Metal-Organic Frameworks and Covalent Organic Frameworks

This effort created novel organic materials with extraordinary functional properties. More specifically, for the first time, single crystals of 2D metal-organic frameworks (MOFs) of sufficient size and quality to enable detailed electrical conductivity measurements were created. This work lays the foundation to understanding the underlying mechanisms in these novel materials necessary for the development of future ultra-low-power, high-efficiency applications in electronics, spintronics, and sensors in support of the Army Modernization Priority of Network Command, Control, Communications, and Intelligence (Network C3I).

CHALLENGE

MOFs are hybrid inorganic/organic materials that are extensively studied for catalysis and gas storage due to their high porosity. However, these materials were not explored as electronic materials, as the vast majority of them are insulators. There are fundamental knowledge gaps in correlating electrical charge transport with porous structures, as well as understanding the mechanism of charge transport. That said, MOFs offer a rich structural and compositional diversity enabled by advances in both organic and inorganic chemistry. If porous, electrically conductive MOFs are created with unique properties, it could open up the possibility of discovering a new platform of materials with extraordinary electronic and magnetic functional properties. Especially interesting in this context are MOFs that form a new class of organic 2D van der Waals (vdW) materials, materials that are made up of layers of single-atom-thick sheets like a stack of paper. The atoms are strongly bonded in the sheet and weakly bonded between the sheets. These materials are expected to have unprecedented properties along with advantages such as scalability, enormous choice of compositions, and access to properties not available in 3D MOFs. However, a fundamental understanding of crystal growth and electrical transport in 2D MOFs was unavailable before the start of this program at ARO.

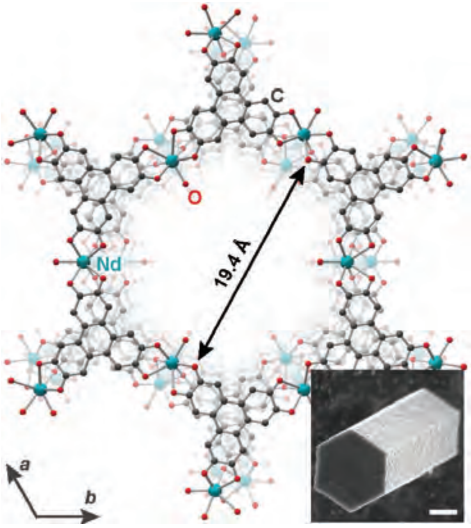


Figure 1: Layered lanthanide MOF [Ln(HHTP)], with a scanning electron micrograph of its large, hexagonal rod crystal. Figure adapted from Skorupskii et al. (2020).

ACTION

In 2016, Dr. Varanasi visited Professor Mircea Dincă's lab at the Massachusetts Institute of Technology (MIT) and had discussions regarding ideas for creating novel conducting organic materials such as covalent organic frameworks (COFs) and MOFs with advanced electronic properties. Professor Dincă proposed to investigate a novel family of 2D MOF materials. His approach included innovative synthesis routes to create single crystals of novel vdW-stacked crystalline 2D MOFs and exploration of the fundamental physical properties (electronic, optical, and magnetic) of these materials. This was a high-risk, high-reward type of work as such materials had never been created before. Dr. Varanasi encouraged a Single Investigator (SI) proposal submission from Professor Dincă and supported this work for three years (2017-2020). At the same time, Dr. Varanasi also approached other chemists in the community and encouraged other efforts following alternate processing approaches and compositions. He initiated a Young Investigator Program (YIP; now Early Career Program [ECP]) with Professor Katherine Mirica at Dartmouth College. She proposed an experimental approach of developing new materials based on conductive 2D COFs and MOFs, and a new paradigm in signal sensing and amplification in solid-state chemical sensors. More specifically, she proposed to synthesize magnetoelectronic COF and MOF materials having stimuli-responsive magnetic and electronic properties.

In collaboration with Dr. Dawanne Poree, the Program Manager for Polymer Chemistry, Dr. Varanasi also started supporting Professor William Dichtel at Cornell University (later moved to Northwestern University) in 2015 through a Multidisciplinary University Research Initiative (MURI) project to explore synthesis and characterization 2D COFs. These strategic efforts in experimental and theoretical work, as well as multidisciplinary efforts via SI, YIP, and MURI vehicles while engaging top scientists have resulted in great advances and discoveries in this field of novel organic materials with extraordinary functional properties.

RESULT

Professor Dincă's work has resulted in synthesizing novel 2D MOFs (Figures 1 and 2) such as nickel hexaiminobenzene [$Ni_3(HIB)_2$], which showed the first signature of metallic behavior in a MOF. He also discovered lanthanide hexahydroxytriphenylene [Ln(HHTP)], which demonstrated that contrary to common understanding, high conductivity in layered MOFs does not require a metal-ligand bond with a highly covalent character, and interactions between organic ligands alone can produce efficient charge transport pathways due to pi stacking (π-π stacking). It was also shown that the electronic structure of conductive 2D MOFs can be reversibly changed by incorporation of gases into the porous MOF structure, as demonstrated on interactions of copper HIB [$Cu_3(HIB)_2$] with carbon dioxide (CO_2) gas. His efforts have shown that vdW materials offer properties that are not realizable with a homogenous structure in these materials systems.

These vdW materials with electrical properties have been shown to be extremely sensitive to external factors such as the presence of gases, which suggests a new platform for next-generation sensors. The Army has always had a need to understand the operating environment with more accuracy and speed. To this end, the future Army will need smaller, more-sensitive, robust, and energy-efficient sensors. One approach is to use 2D MOF materials with unique electronic properties, such as those developed in this effort.

Professor Dichtel's work on 2D COFs has also made significant advances in the synthesis, modeling, and

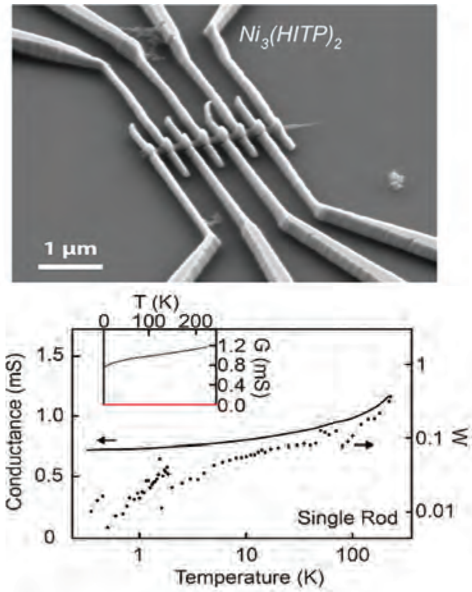


Figure 2: Single-crystal device for a conductivity experiment and plot showing metallic behavior in a 2D MOF. Figure adapted from Day et al. (2019).

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

Results

- Led to publications in *Nature Chemistry, Nature Materials, ACS Central Science*, and *Journal of the American Chemical Society*.
- Led to the hiring of a post-doc at ARL WMRD.

Anticipated Impact

New materials relevant to highly sensitive sensors and other electronic devices are expected to be developed in future.

characterization of these novel materials, and these results were published in high-impact journals (Day et al., 2019; Dou et al., 2020; Feriante et al., 2020; Skorupskii et al., 2020).

Dr. Eric Wetzel and his team members from ARL WMRD collaborated with Professor Dichtel's team in the area of synthesizing COF materials and exploring mechanical properties for the development soft armor for Soldier protection. These interactions have resulted in joint publications and hiring a postdoctoral fellow at ARL WMRD trained in Professor Dichtel's group.

WAY AHEAD

Based on the success of these projects, other 2D MOFs with exotic properties such magnetic, electrical, or optical materials that are responsive to external conditions will continue to be developed. Initial results on electrically conductive 2D MOFs were shared with the Dr. Madan Dubey's team at ARL SEDD and opportunities for initiating new areas of device research were discussed. New devices incorporating these materials will be developed in collaboration with scientists and engineers at ARL SEDD for the applications such as neuromorphic computing and low-power electronics.

This success was made possible by:

Dr. Chakrapani Varanasi, Materials Science Branch

Dr. Sara Gamble, Physics Branch

Dr. T. R. Govindan, Physics Branch

Dr. Frederick Fatemi, ARL SEDD

Citations:

Kim, D. & Englund, D. K. *Science* **363**, 528-531 (2020).

Tian, X. *et al. Nat. Mater.* **19**, 867–873 (2020).

"Penn Engineers Develop Room Temperature, Two-Dimensional Platform for Quantum Technology," *University of Pennsylvania*. (2020).

UCLA-Led Research Team Produces Most Accurate 3D Images of '2D Materials'," *The Graphene Council*. (2020).

SUCCESS STORY

Engineering Defects in Novel Materials for Future Quantum Information Systems

This effort demonstrated novel room-temperature hardware platforms based on 2D materials with engineered defects for possible future use in quantum technologies to support the Army Modernization Priority of Network C3I.

CHALLENGE

Diamonds with engineered defects, such as nitrogen-vacancy color centers, are known to display quantum emission properties that can be easily manipulated by magnetic and electrical fields. These materials have been explored for several decades for application as quantum devices. These investments provided a good baseline to understand basic quantum physics and develop initial demonstrations of possible quantum technologies. However, these diamond-based platforms have limitations mainly due to the difficulty in creating the defects in a controlled fashion, the ability to create an array of qubits at the same depth for uniform sensing, and low coherence times. Future quantum technologies require new material platforms that are more robust, are amenable for scale-up, and offer advanced functionalities that are not currently available such as long coherence time and room-temperature operation. This creates an opportunity to explore other novel material platforms (high-purity, wide-band-gap materials and 2D materials) to address these issues. Two-dimensional materials are appealing because they inherently have all defects on the surface due to being atomically thin, which eases integration into quantum photonic circuits and also there is a wide selection of 2D materials that offer a broad range of optical properties.

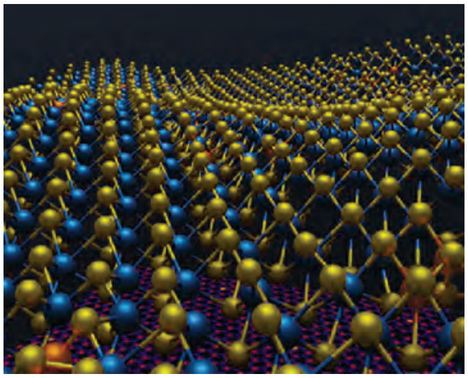


Figure 3: 3D positions of Mo (blue), S (yellow), and doped Re atoms (orange). Figure adapted from *The Graphene Council* (2019).

ACTION

In 2014, Dr. Varanasi had in-depth discussions with Drs. Sara Gamble and T. R. Govindan, who manage programs in quantum information systems (QIS) at ARO, to understand the state of the art of QIS technology and the materials platforms under development at that time to identify needs for innovations in materials to create novel materials platforms. Dr. Varanasi also started discussions with materials scientists in the community who are familiar with novel quantum materials as well as QIS. He visited Professor Lee Bassett at the University of Pennsylvania and had in-depth discussions to identify an opportunity to initiate a program to look for materials that support future QIS. Professor Bassett proposed to investigate point defects (vacancies, impurities, etc.) in wide-band-gap semiconducting 2D vdW materials such as monolayer hexagonal boron nitride (h-BN) and isolate defects with optically addressable spins. Such novel 2D materials (h-BN, molybdenum disulfide [MoS_2], etc.) became available due to ARO's prior investments in this area since 2009 for electronics (see ARO Year in Review from FY18). These 2D materials provide opportunities such as ability to tune and integrate with other devices easily compared with other material platforms. Dr. Bassett proposed that h-BN may have defects similar to nitrogen-vacancy color centers in diamond that can provide room-temperature quantum emission. Dr. Varanasi funded a three-year SI grant in 2015 and a Defense University Research Instrumentation Program (DURIP) grant in 2018 to equip the laboratory to perform the necessary experiments.

Dr. Varanasi also started a two-year SI project with Drs. Konstantin Novoselov and Freddie Withers at the University of Manchester in 2016 to investigate quantum devices based on 2D crystals and their heterostructures. These efforts demonstrated that 2D materials like h-BN and tungsten selenide (WSe_2) have certain natural defects that may be useful for developing future QIS. Dr. Varanasi talked with ARO Program Managers Drs. Gamble and Paul Baker and Dr. Frederick Fatemi at ARL SEDD in 2017, and developed a MURI topic to expand the studies to discover other novel materials and understand the underlying defect physics. A concerted effort that included atomic-scale modeling, synthesis, spectroscopy, and engineering of defects for quantum control was proposed by Professor Dirk Englund of MIT and his team. The MURI was awarded in 2018. This team continues to make significant advances in discovering novel materials such as zinc oxide (ZnO) and WSe_2, and shedding light on novel defects in various novel materials systems.

These strategic efforts, in collaboration with ARO Program Managers and ARL SEDD scientists and engineers, had the foresight to initiate experimental and theoretical efforts through SI, DURIP and, MURI funding vehicles to engage top scientists in materials and QIS, resulting in great advances/discoveries.

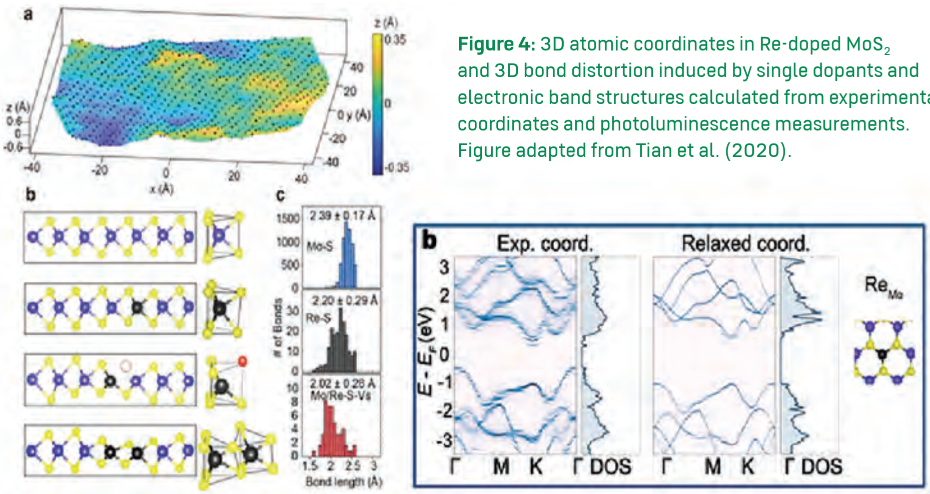


Figure 4: 3D atomic coordinates in Re-doped MoS_2 and 3D bond distortion induced by single dopants and electronic band structures calculated from experimental coordinates and photoluminescence measurements. Figure adapted from Tian et al. (2020).

RESULT

To understand and exploit the novel defects (color centers) in 2D materials, Professor Englund's MURI team developed techniques to image atomic defects in 2D materials with atomic precision by electron tomography. This technique was successfully used to determine the 3D atomic coordinates and defects in rhenium (Re)-doped MoS_2 with picometer precision by a co-principal investigator in the MURI, Professor Jianwei "John" Miao of University of California, Los Angeles (Figure 3). For the first time, experimentally determined 3D atomic coordinates were used by another co-principal investigator in the MURI, Professor Pri Narang of Harvard (a theory expert), as input for density functional theory (DFT) calculations to obtain more-accurate electronic band structures than those derived from conventional DFT calculations that rely on relaxed atomic models (Figure 4). This newly enabled capability to obtain detailed knowledge of the atomic positions is crucial to develop a basic understanding in order to design, predict, and ultimately engineer mesoscopic quantum defects tailored for applications such as quantum memories or nanoscale quantum sensors.

WAY AHEAD

These multiple funded efforts will continue to discover other novel materials (e.g., novel organic, inorganic materials) and defects through characterization, computational modeling, and experimentation. This multifaceted approach is anticipated to yield new materials more suitable for novel quantum technologies that can be operated at room temperature. As these discoveries mature, device designs incorporating these materials will be developed in collaboration Dr. Frederick Fatemi's group at ARL SEDD. Some of the MURI team members already have ongoing collaborations with this team in quantum sciences. With the new collaborations of quantum materials scientists through this MURI, it is anticipated that developing applications in quantum sensing, computing, and communication can be further accelerated.

ARL Competencies:

- Photonics, Electronics, and Quantum Sciences
- Military Information Sciences
- Electromagnetic Spectrum Sciences

Results

- Led to publications in *Nature Materials* and *Science*.
- Led to research collaborations with ARL SEDD.

Anticipated Impact

Novel material platforms continue to be developed with the potential to advance quantum technologies (sensing, communication, and computing) through a paradigm shift: predicting, creating, and controlling materials with atomic certainty.

SYNTHESIS AND PROCESSING OF MATERIALS PROGRAM

Program Manager
Dr. Michael Bakas

Dr. Michael Bakas obtained his Ph.D. in 2006 in Ceramic and Materials Science Engineering from Rutgers University. He worked for nine years at Idaho National Laboratory as a materials researcher.

He arrived at ARO in 2015 as a Systems Engineering and Technical Assistance (SETA) Contractor and in 2017 was appointed Program Manager of the Synthesis and Processing of Materials Program.

Current Scientific Objectives

1 | Define the relationships between processing parameters and material performance to enable the development of qualification procedures for advanced processing methods that, if successful, will enable them to be utilized by the Army for production of high-performance materials for vehicle structures, force protection, and munitions.

2 | Develop a fundamental understanding of the core influences that govern a material's grain structure to enable superior engineering techniques that, if successful, will enable design of enhanced materials for protection or lethality applications.

This success was made possible by:

Dr. Michael Bakas,
Materials Science Branch

Dr. Brandon McWilliams, ARL WMRD

Dr. Elias Jelis, DEVCOM AC

Citations:

"Texas A&M Researchers Uncover the Art of Printing Extremely Hard Steels Flawlessly," *Texas A&M University*. (2020).

Seede, R. *et al. Acta Materialia* **186**, 199-214 (2020).

SUCCESS STORY
Defining Printability for Additively Manufactured Alloys

Two obstacles to the adaptation of additive manufacturing (AM) by the Army are achieving consistent performance and developing qualification procedures. The Synthesis and Processing of Materials Program funded efforts that predicted optimal printing conditions and created new alloys designed for printability, key steps toward enabling AM for Army use.

CHALLENGE

The strength of a metal part is strongly influenced by its alloy composition and the processing method used in its fabrication (e.g., casting and forging). AM-built metallic parts are notorious for their inconsistent performance because of the extreme heat gradient that occurs as the build is created. Changes in the rapid heating and cooling that are inherent to metallic AM processes can lead to flaws such as cracks, voids, or high stresses. Thus, one part may be acceptable, and a second may fail catastrophically. The numerous factors (e.g., speed, alloy composition, and machine design) make it very difficult to link failure to a single cause, creating significant obstacles to the development of qualification procedures that eliminate flawed parts. This limits employment of AM, as there must be confidence a part can perform at the desired level without failing.

ACTION

In 2017, Dr. Bakas did a deep dive into the field of metallic AM, attending conferences and holding discussions with AM experts. He noticed that while the issue of uncertainty and qualification was often mentioned, little work was being done to address it. Most AM efforts presented at conferences and published in journals were focused on attempts to print specific devices using the alloys currently in demand by industry. These alloys are often complex aerospace alloys, making it even more challenging to identify the root causes of inconsistency. A common complaint voiced by researchers was that the AM community is trying to print alloys designed for other fabrication processes, instead of developing alloys designed for AM.

As the Army is investing considerably in the development of AM to address logistical issues and develop components for the next generation of Army equipment, Dr. Bakas decided to direct AM white papers toward questions related to printability. Rather than looking at how to optimize printing given a

Figure 1: Builds of consistently printing steel alloy developed under the STTR. Figure courtesy of Elementum 3D.

specific alloy, he sought to find what an alloy optimized for printability would look like. This would enable researchers to develop new alloys optimized for AM. The ideas these discussions generated enabled Dr. Bakas to use both the Small Business Technology Transfer (STTR) program and Synthesis and Processing of Materials core funds to support research that directly address these questions of printability and consistency.

RESULT

Dr. Bakas worked with Dr. Brandon McWilliams of ARL WMRD to create a STTR topic focused on developing a consistently printable AM metal alloy. The winner, selected in 2018, with input from Dr. Elias Jelis of DEVCOM AC, was Elementum 3D. Elementum proposed working with Professor Aaron Stebner of the Colorado School of Mines (now at the Georgia Institute of Technology), a leader in the AM field, to develop an alloy with a minimal "mushy" zone (the temperature at which the alloy is a mix of solid and liquid). Minimizing this zone should prevent flaws from forming during solidification. The team used machine learning to guide modification of a stainless steel alloy. The result was readily printable with superior mechanical properties to the unmodified alloy (Figure 1). The team is continuing to modify their composition and beginning work on developing a new aluminum alloy. As a result, not only are two new potential products under development, but the rules for creating "printability" in a metal alloy are being established.

Additionally, one of the most successful efforts is being performed at Texas A&M University. In 2018 Dr. Bakas funded a Single Investigator award to a team of researchers, Professors Raymundo Arroyave, Ibrahim Karaman, and Alaa Elwany, to address the task of computationally defining printability. After discussions with Dr. Bakas, the decision was made to work with simplified nickel (Ni) alloys: Ni-neodymium (Nb), Ni-zirconium (Zr), and Ni-aluminum (Al). These compositions are similar to the superalloys used in aerospace, but are easier to predict and study. The team incorporated the various aspects of the printing process into a physics model modified with statistical uncertainty quantification calculations. This framework was used to predict how an alloy would print under various processing conditions, generating a map to optimize processing. The mapping program was adjusted using data gathered from the Ni alloy builds. The computational framework was first used for the printing of Ni-Nb, and work is now proceeding on Ni-Zr and Ni-Al. This map has already been utilized to assist the Air Force in the printing of martensitic steels, reducing the time required to develop the printing process from approximately one year to about one to two months (Figure 2). The framework has attracted interest from industry, with many companies dependent on metallic parts (e.g., petroleum) initiating collaborations with the professors.

By supporting this basic research, the Synthesis and Processing of Materials Program is creating the technical basis for the future development of qualification procedures for AM parts. By defining printability, creating methods to predict it, and achieving it experimentally, the program is addressing the issue of inconsistent performance. This will enable both qualification procedures and commercially available AM optimized alloys for the Army and industry.

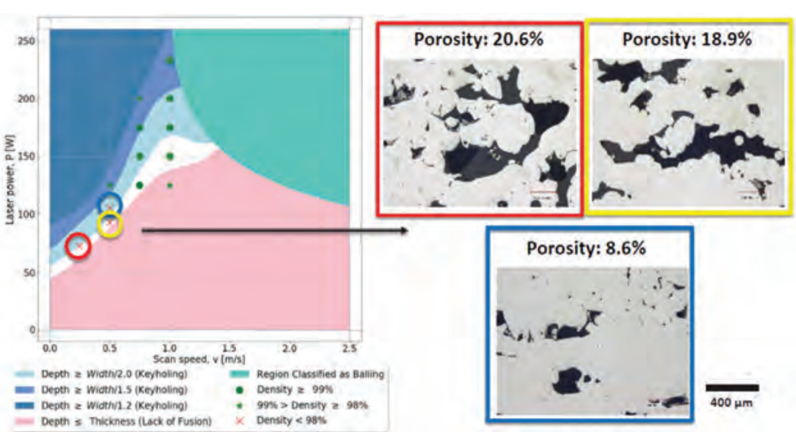


Figure 2: Map of processing conditions for AM to identify region for optimal printing. Figure adapted from Seede et al. (2020).

ARL Competencies:

Sciences of Extreme Materials

Results

- Designed new multi-purpose alloys for consistency under the STTR.
- Created a computational framework for identifying printability windows in metal alloys used to develop a printing procedure for the Air Force.
- Filed a provisional patent for a computational framework for printability prediction.

Anticipated Impact

This computational framework should provide a basis for developing qualification procedures by enabling prediction of the ideal printing parameters for metal alloys. A new family of metal alloys designed for printability should be commercially available for the Army's use in the future, enabling ad hoc solutions to unexpected and acute logistical challenges.

This success was made possible by:

Dr. Michael Bakas, Materials Science Branch

Dr. Efrain Hernandez, ARL WMRD

Citations:

Gupta, A, Zhou, X. & Tucker, G. *Acta Materialia* **190**, 113-123 (2020).

Lu, N. *et al. Acta Materialia* **195**, 1-12 (2020).

Rajaram, S. *et al. JOM* **72**, 1745-1754 (2020).

WAY AHEAD

These efforts are linked to Army research via the collaboration with Drs. McWilliams and Jelis and through the ARL South Regional Center. Phase III STTR opportunities should be leveraged to develop highly printable alloys for more specific Army-relevant needs. The computational framework will be expanded as industry funds the mapping of compositions relevant to their needs.

SUCCESS STORY

Three-Dimensional Digital Characterization of Grain Structures

Grants in the Synthesis and Processing of Materials Program's core program have developed methods of characterizing the process of grain growth and creating 3D representations of a material's grain structure. These methods will enable new methods of further engineering Army-relevant metals and ceramics to obtain superior protection and lethality capabilities.

CHALLENGE

The mechanical properties of ceramics and metals largely determine their performance. These mechanical properties are strongly influenced by the grain structure. Grains are the smaller crystals of the metal or ceramic that when linked together form the bulk material. This network is called the grain structure. The Army is investing in research into materials with nanoscale grain structures in order to obtain superior mechanical properties. Achieving that goal requires understanding both the causes of grain growth and how grains respond to temperature and stress. A nanomaterial that performs well in the lab may fail if the grains grow when stressed. While researchers have theories about the grain growth process, experimental data for these theories is primarily obtained by examining 2D sections of the grain structure via a microscope. Methods that can observe the grain growth as it occurs and properly represent the structure in 3D are needed to refine and validate grain growth models.

ACTION

In 2018 Dr. Bakas attended a workshop at University of California, Irvine focused on addressing some of the outstanding challenges in nano-grained materials. What emerged was a lack of clarity on many of the potential mechanisms relevant to controlling grain size. To address this issue, Dr. Bakas encouraged studies into capturing the relevant phenomena in situ. The solutions the researchers developed led to compelling new methods for capturing and displaying the process of grain growth in 3D.

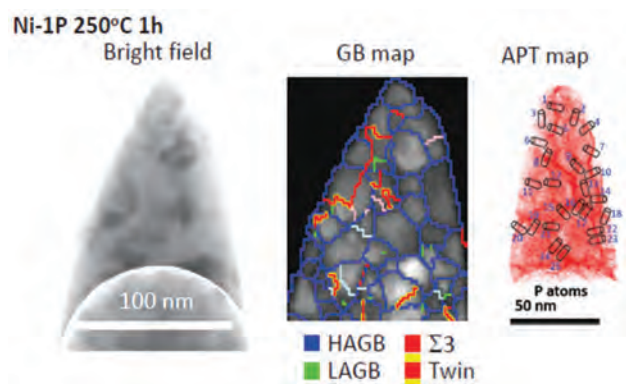


Figure 3: TEM characterization of the grain structure in a nanocrystalline Ni-1P alloy. Figure adapted from Gupta et al. (2020).

RESULT

The University of Alabama and Colorado School of Mines are collaborating on a Single Investigator award to study the response of nanostructures to mechanical stress by linking experimental results (University of Alabama) with computational modeling (Colorado School of Mines). To observe the nanograins while under stress, the University of Alabama developed a new testing apparatus for a transmission electron microscope (TEM) that allowed mechanical testing at elevated temperatures in the TEM (Figure 3). This enabled imaging of nanosized grains as they responded to the stress. The Colorado School of Mines used that data to calibrate a digital reconstruction of the tests. Once digitized, the now-digital grain structure could be virtually tested using the simulation to evaluate its response to other types of stress. Initially, these reconstructions had to be viewed on a monitor, but the Colorado School of Mines became aware of a virtual reality (VR) program for medical research at Colorado State University. The grain structure data was provided to Colorado State, who implemented it into their VR system, allowing a researcher to directly examine the grain structure in 3D (Figure 4). This is significant as the shape of the grain often has a strong influence on its growth, and it is much easier to understand that influence when viewing in 3D. The University of Alabama has an ongoing collaboration with ARL WMRD, co-publishing papers together on ARL's in-house efforts in nanocrystalline alloy development. This existing collaboration positions the Army to benefit from this characterization method.

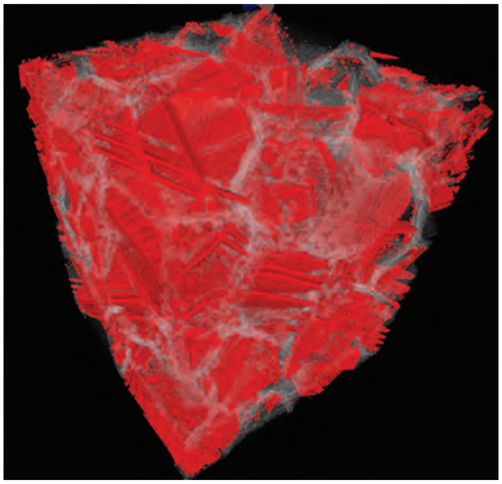


Figure 4: Digital reconstruction of the grain structure viewed in VR. Figure adapted from Rajaram et al. (2020).

Another effort that has made considerable progress is a Young Investigator Program (now Early Career Program [ECP]) grant performed by Professor Ashwin Shahani of the University of Michigan. Professor Shahani combined two different x-ray imaging techniques into a unified method that allowed him to capture the evolution of a grain structure during heating. Using an Al-copper (Cu) alloy as a test case, Professor Shahani did a 97-min hold at 485 °C, and watched as one grain grew large and consumed all others. Using this tool, Professor Shahani can now study grain growth as it occurs at high temperatures. The data generated by the x-ray imaging can be used to create digital 3D representations, allowing a researcher to review the experiment at any time and from any angle (Figure 5). Professor Shahani recently linked up with Dr. Efrain Hernandez of ARL WMRD to provide his data to support Dr. Hernandez's own simulations of grain structure evolution. These advances in simulation, characterization, and representation of grain growth have the potential to enable the development of advanced materials with extraordinary strength by enabling an unprecedented level of control of the grain structure.

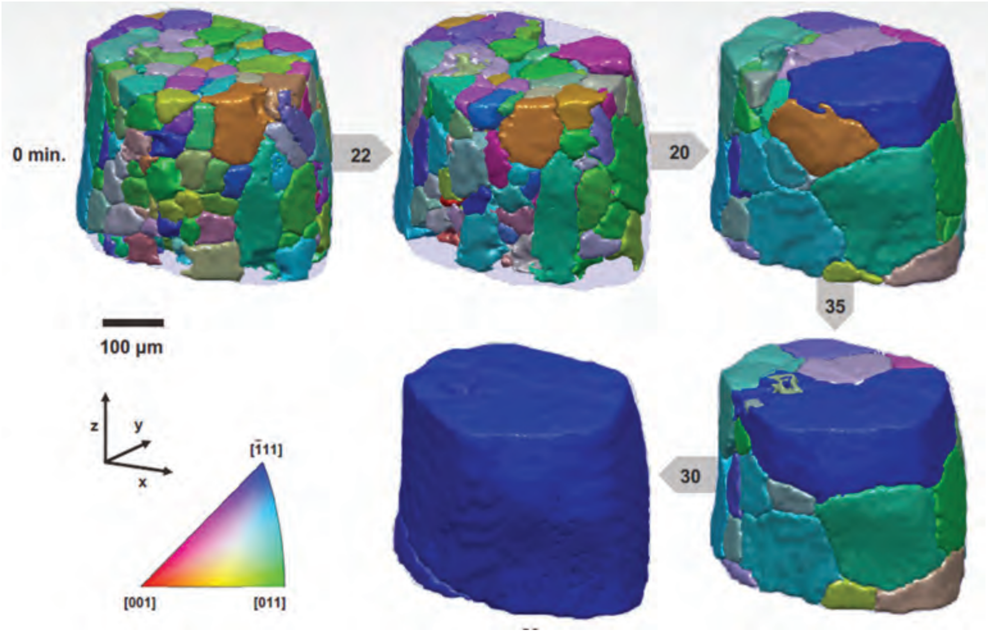


Figure 5: X-ray imaging of Al-Cu alloy during a 97-min anneal at 485 °C. Figure adapted from Lu et al. (2020).

WAY AHEAD

These new characterization tools will be leveraged to support ARL's in-house research efforts for nanoscale alloy development. This will be accomplished through continued collaborations with ARL WMRD. As knowledge of the fundamental mechanisms controlling grain structure are better understood, it should be possible to both stabilize nanostructured materials and create materials with specific grain distributions engineered for optimum performance for use in vehicles and protective systems.

ARL Competencies:

Sciences of Extreme Materials

Results

- Led to co-publication between WMRD and the University of Alabama in *Acta Materialia* and *Applied Physics Letters*.
- The University of Alabama developed a characterization method, now used as an ARL procedure for characterizing internally developed alloys.
- Demonstrated the use of a VR system for viewing grain structures at The Minerals, Metals and Materials Society conference.

Anticipated Impact

These new methods of characterizing and viewing grain structures should enable the engineering of grain structures that provide to superior mechanical properties. These advanced materials could contribute to advanced armor and weapon systems for the Army.

COMPLEX DYNAMICS AND SYSTEMS PROGRAM

Program Manager Dr. Samuel Stanton

Dr. Stanton completed his undergraduate studies at the U.S. Naval Academy, receiving his B.S. in Aerospace and Astronautical Engineering in 2004. He completed his graduate training at Duke University, receiving his M.S. and Ph.D. in Mechanical Engineering in 2008 and 2011, respectively.

He came to ARO in 2011 as the Program Manager for the Complex Dynamics and Systems Program and additionally served as Acting Program Manager for Multi-Agent Network Control for several years.

Current Scientific Objectives

1 | Discover, predict, infer, and control the most important dynamic features of high-dimensional nonlinear systems that, if successful, could lead to a massive change in DoD tools to perform design, make inferences from data, and control complex systems.

2 | Determine the principles by which agile and adaptive cognition, computation, and control is physically encoded within organisms and machines that, if successful, will enable robotic Soldier squad augmentation capable of keeping pace with high op-tempo operations in all terrain types.

3 | Discover how the geometric structure underlying information processing and control modulate the non-equilibrium statistical mechanics of low-to-infinite-dimensional stochastic dynamical systems that, if successful, will lay the foundations for a broad range of systems such as nanoscale systems capable of coordinating molecular assembly of materials and systems with novel properties for modular robotics and reconfigurable assemblages of autonomous swarms or novel micro-architected structures with distributed actuation, vibration protection, and shock mitigation for both ground and air vehicle technologies.

This success was made possible by:

Dr. Samuel Stanton, Mechanical Sciences Branch

Dr. Denise Ford, Mechanical Sciences Branch

Dr. Marc Ulrich, Physics Branch

Citations:

Fruchart, M., Zhou, Y. & Vitelli, V. *Nature* **577**, 636-640 (2020).

Lerner, L., "UChicago Scientists Push the Boundaries between Materials and Machines," *University of Chicago*. (2020).

Scheibner, C. *et al*. *Nat. Phys*. **16**, 475-480 (2020).

SUCCESS STORY

Active Structures Bridging Mechanics and Computation

This effort opened entirely new doors to future adaptive structures capable of manipulating and storing information in vibrational waves the same way advanced quantum computation technologies use the charge and spin of electrons. Research results may be a first step toward a new field of "mechanical spintronics" leading to structures capable of intelligently mitigating unwanted vibration and noise in air and ground vehicles.

CHALLENGE

Can structures be redefined by merging mechanics and computation? The goal of this research is to create mechanical systems that serve as both hardware and software to perform elaborate information processing tasks. For example, when an elastic beam bends, it performs a very simple computation. The input of this primitive computer is the load, while its output is the deflection of the beam. However, the shape of an elastic material can encode much more information, enough to encode the result of a useful computation. Is it possible to write a computer program into the microscopic structure of a material so that it is executed when the material is perturbed (e.g., mechanically deformed)?

ACTION

Dr. Stanton created new opportunities in structural control by initiating workshops bringing together experts in mechanics, materials, and physics working on the state of the art in engineering structures, metamaterials, and the physics of active matter. He identified an opportunity to merge these disciplines in Army-relevant directions by focusing on how these fields can merge to introduce the concept of metastructures: micro-architected active lattices with behavior that may be highly influenced by their finite extent and their overall shape, dimensions, and boundary/interface conditions.

New and potentially very high-impact scientific results extending the field of topological mechanics to elasticity and computation were presented at the workshop by Professor Vincenzo Vitelli of the University of Chicago. Dr. Stanton reached out to Professor Vitelli to begin a conversation on how the centuries' old field of elasticity in mechanics should adapt to consider actuation at the smallest length scales and how the similarities in the topological properties of electro-optical systems could be exploited in mechanical systems. Dr. Stanton also invited Professor Vitelli to give a talk at ARO to facilitate cross-disciplinary opportunities between his program and the Physics Branch at ARO. Professor Vitelli then crafted a proposal to address fundamental questions that were discussed at length with Dr. Stanton and several ARO Physics Branch program managers, leading almost immediately to several high-impact scientific breakthroughs.

RESULT

Professor Vitelli's new research efforts, supported by ARO with a Single Investigator award in 2019, introduced the new field of odd elasticity and a new understanding of how abstract mathematical features of dynamic systems could inform next-generation mechanical computation. A mechanical structure that computes must be active. However, there was no formal theory of elasticity that could handle non-equilibrium (active) systems. Professor Vitelli successfully formulated a universal theory of active elasticity called odd elasticity. This led to one of the first papers published in the prestigious journal *Nature Physics* on pure mechanics in decades (Scheibner et al., 2020).

Bridging the electro-optical properties of matter with mechanics was accomplished by leveraging the deep mathematical connections between unrelated systems called dualities. In mathematics, the idea of symmetries and their breaking are the cornerstone of a physical understanding of natural phenomena. However, to realize future synthetic structures capable of intrinsic computation and control, research must reach beyond nature and no longer rely on symmetries. By instead studying dualities in the mathematics of structures, new opportunities were discovered to create unique properties: hidden symmetries in the mechanical response and, most intriguingly, new abilities to use vibrational waves in the same way quantum computation uses electron spins (Figure 1). This latter advance establishes novel paradigms for materials that compute. More broadly, though, this work illustrates the power of duality relations in mechanics and wave physics. The investments in this aspect of the program may play as crucial a role in the design of future mechanical metamaterials.

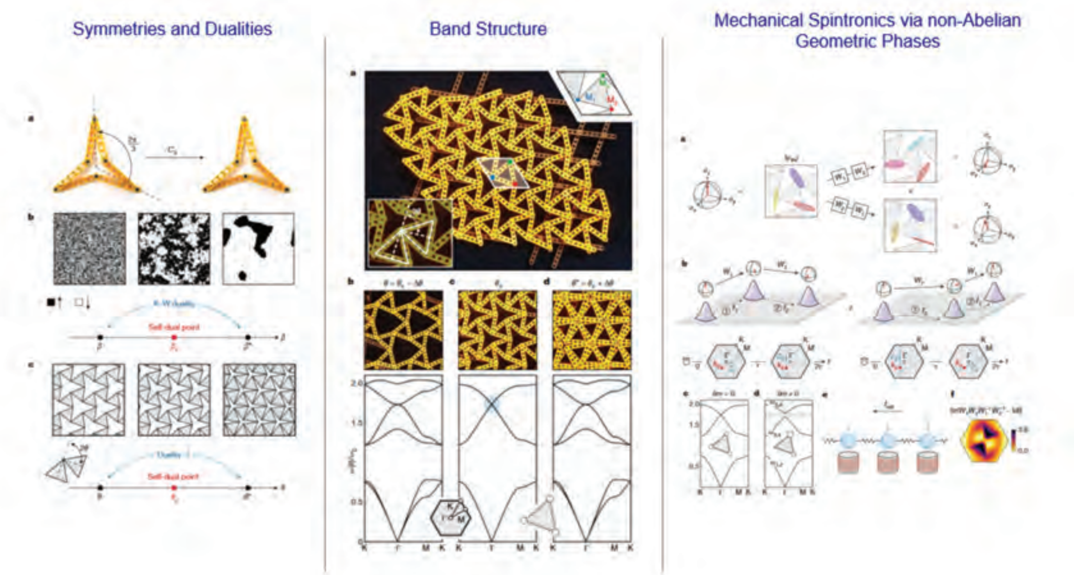


Figure 1: Symmetries and dualities in mechanical systems. (Left) A symmetry is a transformation that maps a system onto itself, as seen by the rotation acting on this structure. A duality, on the other hand, relates these models or structures. The order–disorder duality between low- and high-temperature phases of the Ising model is a classic example. There exists a temperature and a dual temperature with a critical phase transition temperature between ferromagnetic and paramagnetic domains. The same phenomena can occur in a twisted lattice mechanical system. As rotation angle is varied, in this setup, a dual mechanical structure can be realized, which is another twisted lattice with a strong relationship to the dynamics of the initial orientation. (Middle) Such dualities can be harnessed to engineer unique static and dynamic properties. Comparing of the lower panels of this figure reveals that two lattices related by a duality transformation share the same band structure despite their clear structural differences. (Right) Non-Abelian sound waves can arise in self-dual mechanical structures, suggesting that energy and thus information can be localized in momentum space by constructing wave packets that are effectively carrying one qubit of information. This is effectively now topological quantum information processing in a completely classical regime and hence "mechanical spintronics" for computation. Figure and caption adapted from Fruchart et al. (2020).

ARL Competencies:

Sciences of Extreme Materials

Mechanical Sciences

Results

- Developed a new framework for odd elasticity that is being transitioned to and adapted by ARL researchers for future structural active matter.

Anticipated Impact

Advances in odd elasticity and dualities are expected to enable future leap-ahead technologies such as mechanical structures capable of computing and possibly even instantiating concepts in machine learning.

WAY AHEAD

In 2020 Dr. Stanton linked Professor Vitelli's research group with Drs. Bryan Glaz and Adam Svenkeson of ARL to help inform approaches to the problem of structural active matter (i.e., matter that can intrinsically reconfigure using both energy and information as well as serving a structural function). Ensuing research discussions have specifically focused on extending Professor Vitelli's approach to odd elasticity to disordered systems to bridge the underlying science with biology and the mechanics of muscles. This could lead to new types of actuating structures for a ground and vehicle platforms.

This success was made possible by:

Dr. Samuel Stanton, Mechanical Sciences Branch

Dr. Robert Kokoska, Life Sciences Branch

Citations:

Ilton, M. *et al. Science* **360**, EAA01082 (2018).

SUCCESS STORY

Understanding and Engineering Extreme Actuation in Future Robotics

This effort established a complete framework spanning biology, materials, dynamics, and controls for extreme actuation inspired by nature's most explosive movements. This will lead to extreme dynamic and reactive movements of future robotic systems.

CHALLENGE

A multitude of organisms across length scales and species use physiological specializations capable of extremely rapid and recoverable movements. In some cases, forces are generated with accelerations exceeding millions times that of gravity within a matter of nanoseconds—outperforming by orders of magnitude our best artificial capacities for repetitive motion. Mechanical power limitations in motors/muscles and springs emerge from the inextricable, physical tradeoff between force and velocity. The underlying science in fast biological force generation, however, has remained fragmentary and synthetic emulation of animal movement has focused on slow, rhythmic dynamics. Lack of a principled, systems-level understanding has led researchers attempting to artificially achieve fast, impulsive dynamics to pursue irreversible energy conversion (e.g., through detonation of energetic materials). New, multidisciplinary approaches are necessary to develop fundamental principles governing interactions between the chemical, physical, and biological mechanisms sustaining exceptional elastic energy storage and rapid release.

ACTION

Dr. Stanton developed a Multidisciplinary University Research Initiative (MURI) topic to establish the necessary scientific principles to guide the future toward solutions for highly reactive autonomous systems. Most academic responses believed the solution lies in buckling or snap-through devices. However, in 2015, Dr. Stanton selected a team with a completely different but extremely well-motivated approach inspired by the real behavior and physiology of small organisms. The team was led by Professor Sheila Patek of Duke University with leading researchers in biology, robotics, and materials scientists. The cornerstone of their approach to establish the principles governing extreme actuation in both nature and machines lies in the ubiquitous evolutionary solution of latch-mediated-spring actuation (LaMSA). LaMSA systems behave similarly in principle to an archer operating a bow and arrow: researchers discovered that the combination of elastic recoil and latch mediation take advantage of and overcome energetic losses to achieve extraordinarily precise movements with high power density. This is distinct from usual approaches for impulsive force generation based on buckling phenomena.

However, Dr. Stanton emphasized the critical need for repeatable motion. Fortunately, being repeatable is a distinctive feature of natural LaMSA systems, but fundamental understanding is crucially hampered by the limitations of current mathematical frameworks. The dynamics of LaMSA systems are highly nonlinear due to the nature of the energy storage mechanism, the kinematics of the articulated linkages, and the often discontinuous nature of making and breaking contact in latch mechanisms. This results in challenges for applying traditional reactive or model-based predictive control techniques to either reject external perturbations or achieve a targeted state in the presence of uncertainty.

RESULT

The research team discovered that power enhancement emerges through dynamic coupling of motors, springs, and latches, each of which displays its own force–velocity behavior. Their first full-team paper mathematically defined a rich and tunable performance space for spring-actuated movement that is equally applicable to biological and synthetic systems (Figure 2; Ilton et al., 2018). The team identified critical transitions in mass and tradeoffs in spring scaling—both of which offer alternative explanations for long-observed scaling patterns in biological systems. Integrating mathematical,

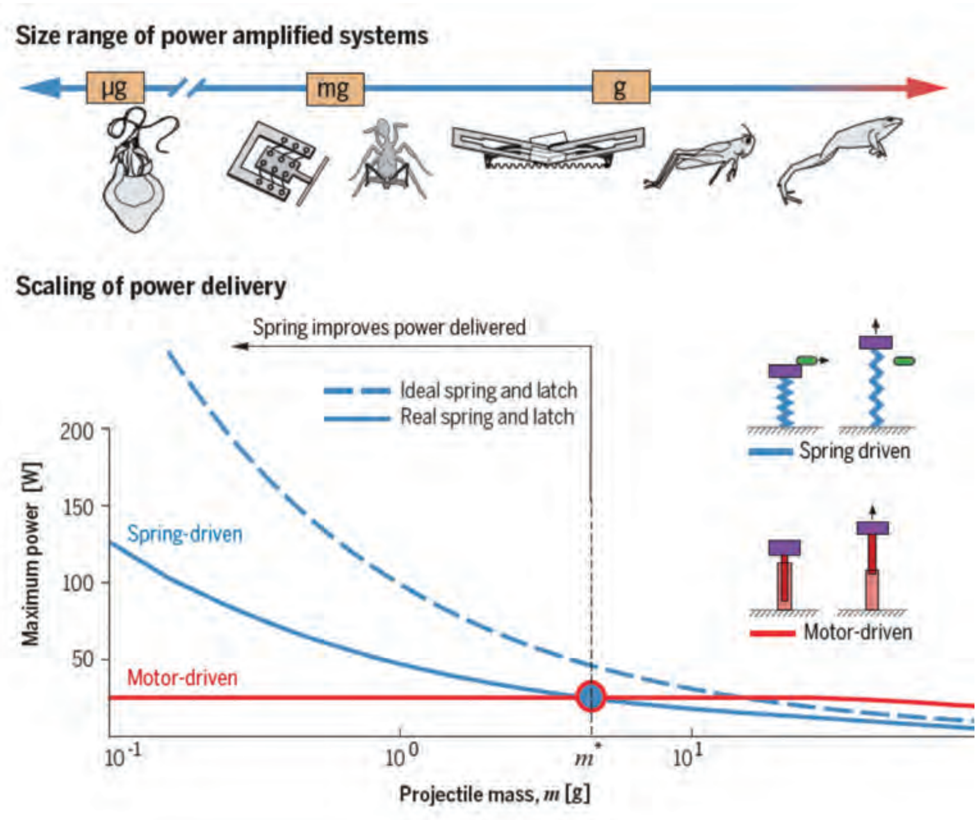


Figure 2: Power-amplified biological and synthetic systems use spring elements to drive motion over a range of size scales. Mathematical modeling reveals a cascade of power limits and mass-dependent transitions in power delivery that arise from the integration of motors, springs, and latches to actuate movement. Variation of these components creates synergistic effects relevant to the analysis and synthesis of diverse power-amplified systems. Figure adapted from Ilton et al. (2018).

physical, engineering, and biological approaches illuminated cascading challenges of power enhancement and their emergent effects in biological and engineered systems. Importantly, this study also pinpointed a specific blind spot for studies of power enhancement: the experimental analysis of power output by non-motor actuators (i.e., springs).

A new interdisciplinary paradigm for closed-loop LaMSA control was also introduced. In the past, such systems were believed to operate only in open loop. New control theoretical approaches were established to identify how the unique properties of the components of LaMSA systems instantiate feed-forward and feedback control.

WAY AHEAD

The underlying science will guide the integration of extreme movement into the design of future robotic systems with the potential to produce more agile and powerful robots.

ARL Competencies:

Sciences of Extreme Materials

Mechanical Sciences

Results

- Discovered the principles of cascading power limits in small, fast biological and engineered systems.

Anticipated Impact

Fundamental understanding of biologically inspired motion such as LaMSA is expected to enable future leap-ahead technologies such as reactive and highly agile robotics.

EARTH MATERIALS AND PROCESSES PROGRAM

Program Manager
Dr. Julia Barzyk

Dr. Barzyk completed her undergraduate studies at the University of Rochester, receiving her B.A. in Geology in 1998. She received an M.S. in Geological Sciences from the University of Florida in 2000 and an M.S. in Environmental Science and Policy from the University of Chicago in 2002. She received her Ph.D. in Geophysical Sciences from the University of Chicago in 2007.

She came to ARO in 2015 as the Program Manager for Earth Materials and Processes.

Current Scientific Objectives

1 | Determine how grain-scale features influence bulk properties in unconsolidated earth materials that, if successful, will enable rapid and accurate simulation of vehicle–terrain interaction.

2 | Develop methods to remotely determine earth surface properties that, if successful, will enable unmanned reconnaissance to inform routing decisions or tracking enemy movements.

3 | Enable prediction of earth surface interaction with air and water at Warfighter-relevant spatiotemporal scales (microns to 100s of kilometers) that, if successful, may provide advance notice of environmental hazards ranging from contaminant dispersal in dense urban environments to brownout in arid regions.

This success was made possible by:

Dr. Julia Barzyk, Mechanical Sciences Branch

Citations:

Seiphoori, A., Ma, X.-G., Arratia, P. E. & Jerolmack, D. J. *Proc. Natl. Acad. Sci. USA* **117**, 3375-3381 (2020).

Unger Baillie, K., "Looking to Mud to Study How Particles Become Sticky" *Penn Today*. (2020).

SUCCESS STORY
Solid Bridging to Explain Fine-Particle Aggregation

A collaboration between geophysicists and mechanical engineers led to discovery of a "sticking" mechanism in fine particles, such as clays that make up mud. This research may lead to new approaches to manufacturing using indigenous materials and aid in modeling vehicle–terrain interaction. This research was made possible through an initiative in Dr. Barzyk's program to use approaches and tools developed in other disciplines to study earth materials and geoscience phenomena.

CHALLENGE

The study of earth materials is challenging due to the extreme heterogeneity and complexity, which has made it difficult to study how grain-scale features influence bulk behavior. Modeling of systems involving sand-sized particles (100s of micrometers) has been accomplished, as these particles are inert. However, in the case of smaller particles (1-10s of micrometers), electrostatic forces are thought to play an important role in inter-particle interactions, making these particles more difficult to study. For this reason, geoscientists and geotechnical engineers have typically relied on empirical studies of earth materials behavior.

ACTION

In 2015, Dr. Barzyk began an initiative to support research efforts that partner a geoscientist with a scientist or engineer from another discipline. Partnerships that involved researchers from the same university were targeted, as this allows students and postdocs to be jointly mentored and perform a truly interdisciplinary project. To make this effective, Dr. Barzyk funded these awards at "double" the normal level to support each researcher and ensure that effort was equally drawn from both disciplines. In this case, Dr. Doug Jerolmack, a geoscientist who had been funded by ARO previously on geoscience topics, partnered with Dr. Paolo Arratia, a mechanical engineer, who is an expert in colloidal suspensions and had not previously worked on earth materials. Both are at the University of Pennsylvania.

RESULT

The team used an experimental approach to study what controls the strength and stability of an aggregate. The results of this approach were highlighted earlier this year in an article from *Penn Today*, "Looking to Mud to Study How Particles Become Sticky" (Unger Baillie, 2020):

They suspended glass spheres of two sizes, 3 microns and 20 microns, in a droplet of water. For reference, a human hair is roughly 50 to 100 microns in width. As the water evaporated, the edges of the droplet retreated, dragging the particles inward. Eventually the shrinking water droplet transformed into multiple smaller droplets connected by a thin water bridge, known as a capillary bridge, before that, too, evaporated.

The team found that the extreme suction pressures caused by evaporation pulled the small particles so tightly together that they fused together in the capillary bridges, leaving behind solid bridges between the larger particles, to which they also bound, once the water evaporated completely.

When the team rewet the particles, applying water in a controlled flow, they found that aggregates composed solely of the 20-micron particles were much easier to disrupt and resuspend than those composed of either the smaller particles, or mixtures of small and larger particles.

In addition to these results, the research team discovered that particles greater than 5 microns were much less stable when rewet than particles less than 5 microns. This caused the principal investigators to question what the effect of mixed particle sizes would be:

In further tests with mixtures of particles of five different sizes—more closely mimicking natural soil composition—the researchers found the same bridging effect at different scales. The largest particles were bridged by the second largest, which were in turn bridged by the third largest, and so on. Even mixtures that contained only a small fraction of smaller particles became more stable thanks to solid bridging.

To determine how much more stable, the team turned to new capabilities in very-high-resolution analysis where an atomic force microscope probe was glued to a single particle, set, and then the "pull-off force" required to remove that particle from the aggregate was quantified: "Repeating this for particles in aggregates of both big and small particles, they found that particles were 10 to 100 times harder to pull off when they had formed a solid bridge structure than in other configurations" (Figures 1 and 2). Thus, leading to a final set of experiments (Figure 3):

To convince themselves that the same would be true with materials besides their experimental glass beads, they performed similar experiments using two types of clay that are both common components of natural soils. The principles held; the smaller clay particles and the presence of solid bridges made aggregates stable. And the reverse was also true. When clay particles smaller than 5 microns were removed from the suspensions, their resulting aggregates lost cohesion.

WAY AHEAD

The study of vehicle–terrain interaction, or terramechanics, is critical to design and manufacturing of new ground vehicles as well as routing of existing vehicles. DEVCOM GVSC is the leader in the development and application of terramechanics, and is leading development of a new approach to modeling these interactions that relies on grain-scale interactions. These models so far can accurately model the behavior of larger particles but, to date, have not incorporated the cohesive effects that arise from the presence of small particles, which are abundant in soils. These new findings have been shared with DEVCOM GVSC at a workshop held in 2019. These results also contributed to motivation for a larger Multidisciplinary University Research Initiative (MURI) effort to be developed on fine-particle interactions, which is currently in competition. The MURI is being followed by scientists and engineers from ARL, the Air Force Research Laboratory, the Office of Naval Research, and Los Alamos National Laboratory.

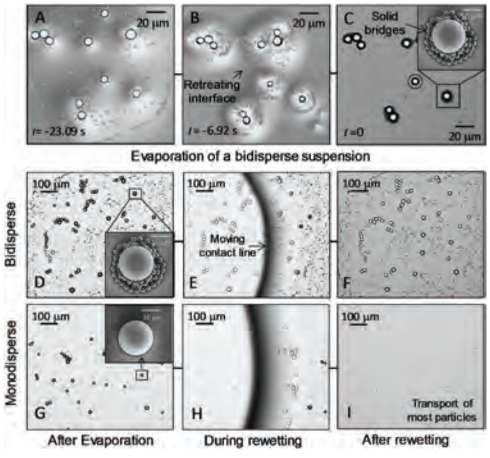


Figure 1: Contribution of solid bridges to stabilizing the evaporation-induced aggregates. (A and B) Evaporation from a bidisperse suspension comprising 20- and 3-µm silica spheres, where smaller particles condense within the diminishing capillary bridges. (C) Formation of solid bridges between larger particles or between particles and the substrate. A higher magnification of an aggregate formed by solid bridges is presented in the inset. (D–F) Stability of aggregates due to the presence of solid bridges. An isolated aggregate is shown in the inset of photomicrograph D under higher magnification. (G–I) Transport of 20-µm particles in the absence of smaller particles and the associated solid bridges. An isolated particle is shown in the inset of photomicrograph G under higher magnification. Figure and caption adapted from Seiphoori et al. (2020).

ARL Competencies:

Sciences of Extreme Materials

Mechanical Sciences

Results

- Published an article in *Proceedings of the National Academy of Sciences*.
- Discovered a new explanation for cohesion.
- Led to further exploring of potential implications for terramechanics.

Anticipated Impact

The new explanation for particle cohesion is expected to enable future leap-ahead technologies such as modeling vehicle terrain interaction and use of indigenous materials.

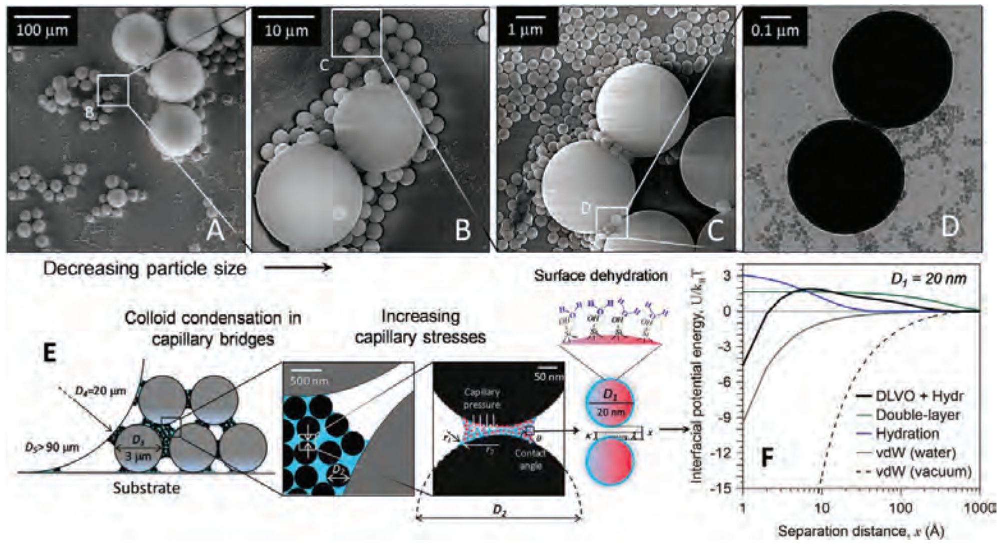


Figure 2: Hierarchical structure of aggregates. (A–D) Multiscale observation of a polydisperse colloidal system comprising silica spheres with particle sizes of 90, 20, 3, and 0.4 µm along with silica nanoparticles of 20-nm size. (E) Capillary force drives particles together by overcoming the inter-particle repulsion. Further dehydration of the particle surface is energetically favorable, resulting in an overall van der Waals (vdW) attraction between particles. (F) Interfacial potential energy functions between two particles of D1 = 20-nm size, calculated from theory. Figure adapted from Seiphoori et al. (2020).

This success was made possible by:

Dr. Julia Barzyk, Mechanical Sciences Branch

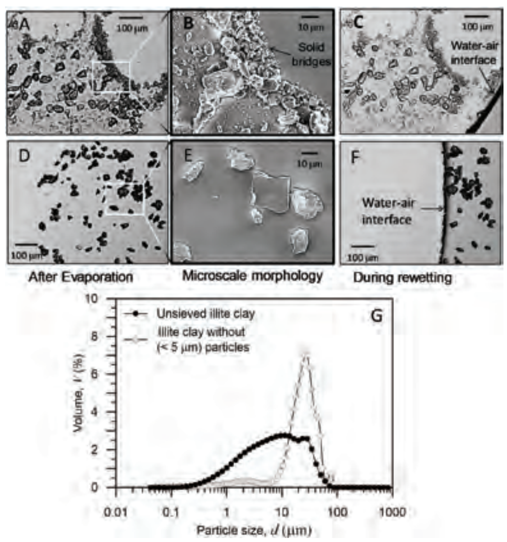


Figure 3: Stability of aggregates of illite clay particles through formation of solid bridges. (A) Aggregates formed by unsieved, polydisperse illite particles. (B) Morphology of the solid bridges at microscopic scale. (C) Aggregates are stable when subject to rewetting, due to solid bridges. (D) Aggregates of same illite clay modified by sieving out particles of less than 5 µm. (E) Morphology of illite particle deposits. (F) Removal of small particles makes aggregates unstable in reaction to rewetting. (G) Particle size distributions of unsieved and sieved illite particle suspensions. Figure adapted from Seiphoori et al. (2020).

SUCCESS STORY

Particle-Scale Tracking and Bulk-Scale Modeling of River Sediments

A collaboration between geophysicists and mechanical engineers led to a new method to track "real" river gravel and use grain-scale data to inform models of bulk material behavior. This research was made possible through an initiative in Dr. Barzyk's program to use approaches and tools developed in other disciplines to study earth materials and geoscience phenomena, and has inspired an application to armor.

CHALLENGE

Historically, the way to describe and predict sediment transport was to use empirically derived formulas for the average bulk rate of transport for the average flow of a stream. These average bulk values were used because no one had been able to measure and model the physics underlying particle motion in natural real-world flows. Because of the irregular grain shape of natural river gravel, grain-scale tracking during flume experiments using these particles is very technically challenging. Further, within the geoscience community, there was no existing method to use grain-scale data to inform bulk material behavior; that expertise would have to come from other field.

ACTION

As described previously, in 2015, Dr. Barzyk began an initiative to support research efforts that partner a geoscientist with a scientist or engineer from another discipline. Partnerships that involved researchers from the same university were targeted, as this allows students and postdocs to be jointly mentored and perform a truly interdisciplinary project. To make this effective, these awards were funded at "double" the normal level to support each researcher and ensure that effort was equally drawn from both disciplines. In this case, Dr. Taylor Perron, a geoscientist who had been funded by

ARO previously on geoscience topics, partnered with Dr. Ken Kamrin, a mechanical engineer, who is an expert in continuum modeling and had not previously worked on earth materials. Dr. Barzyk introduced these researchers to each other when it became apparent that the continuum modeling Dr. Kamrin develops could be applied to earth materials. Both are at the Massachusetts Institute of Technology (MIT). These ideas were developed into a Single Investigator proposal, which was funded as a proof-of-concept study in 2015 to demonstrate that gravel tracking could be achieved. After the success of that effort, a larger award was made in 2017.

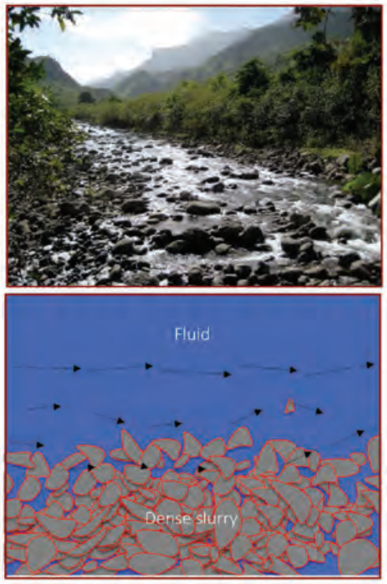


Figure 4: River gravel transport; the top image is the Fraser River in British Columbia, Canada. Figure courtesy of Drs. Perron and Kamrin.

RESULT

This effort was aimed at understanding the physics of particle motion and involved numerical simulations and flume experiments performed simultaneously and integrated so that they would be most valuable. The flume was designed to simulate river flow, and the first experiments were performed using glass spheres. These experiments were performed at Simon Fraser University in Vancouver in a collaboration with Dr. Jeremy Vendetti.

In the 18-month preliminary effort, the team demonstrated that they could track spheres. Once this method was developed, they moved on to the more challenging task of tracking natural grains. Real gravel grains from the Fraser River in British Columbia were used (Figure 4), and the grains were painted in eight different colors to enable the tracking process, which used high-speed video capturing hundreds of frames per second. A machine learning algorithm was developed with the help of some computer science undergraduate students at MIT, in which code that had been written to identify street signs was modified to perform the grain tracking.

In addition to tracking the individual grains and determining the grain velocities from this method, the team also measured the fluid velocity both in the fluid field overall and around the individual grains using particle image velocimetry and laser Doppler anemometry, respectively. This is very important data to get from the experiments because these are the velocities that are calculated in the numerical simulations, and therefore, enable direct comparison between the simulations and the experiments.

For the simulations, a discrete element method (DEM) model was used to model the interaction of particles with each other and then this was coupled to a lattice Boltzmann method model, which models the fluid phase—a fully custom code that is based on the experiments. A significant advantage of this approach is that these results can be matched to the conditions observed in the flume experiments, in terms of overall fluid field as well as around individual grains; this was the first time that flow around and between the grains had been accomplished in these types of experiments.

WAY AHEAD

The next step of this effort is to perform the numerical simulations for the natural grains. To do that, computed tomography (CT) scans of river gravel are performed and, using an existing DEM code, the natural gravel is approximated by fitting the contours of the non-uniform shape with a series of overlapping spheres. Current efforts are trying to determine how to most efficiently approximate natural gravel while balancing accuracy with speed. When this work is complete, a continuum model, based off of grain-scale physics, will provide, for the first time, an alternative to empirical sediment transport models. These results may lead to new approaches to erosion control, siting and maintenance of infrastructure, and land management.

Dr. Kamrin has begun a new collaboration with Dr. George Gazonas of ARL WMRD on the topic of discrete and continuum impact modeling, and ARL WMRD has invested in further development of these modeling approaches through the Institute for Soldier Nanotechnology (ISN) at MIT (a University Affiliated Research Center [UARC]) to help understand ceramic damage during impact through the use of models of bulk material behavior informed by particle-scale dynamics, as the strength of ceramics depends largely on the hydrostatic pressure, with more tightly confined samples experiencing higher strength throughout the damage process. While experiments have been able to characterize the response within certain levels of confining pressure ($\leq$ 40 GPa), larger confining pressures are harder to maintain in experimental tests. The team's DEM representation could be a stand-in for experiments and allow, in a controlled fashion, simulated probing of the high-pressure fully damaged response of ceramic materials, with applications to high dynamic loading.

ARL Competencies:

Sciences of Extreme Materials

Mechanical Sciences

Results

- Published articles in journals including *Proceedings of National Academy of Sciences* and *Journal of Fluid Mechanics*.
- Developed the first method to track natural grains in flume experiments.
- Led to a new collaboration with ARL WMRD on ceramic damage processes during impact.

Anticipated Impact

This study of sediment transport in river and the associated particle and continuum-scale modeling is expected to enable future leap-ahead advances in our understanding of impact-related damage processes and erosion processes.

ESD Engineering Sciences Division

Electronics Branch | Materials Science Branch | **Mechanical Sciences Branch**

FLUID DYNAMICS PROGRAM

Program Manager
Dr. Matthew Munson

Dr. Munson completed undergraduate studies at the Illinois Institute of Technology, receiving a B.S. in Aerospace Engineering in 2002. He pursued doctoral studies at the California Institute of Technology, receiving a Ph.D. in Aeronautics in 2012.

A recipient of both the DoD National Defense Science and Engineering Graduate (NDSEG) Fellowship and the Science, Mathematics and Research for Transformation (SMART) Scholarship, Dr. Munson started at ARL in 2012 as an aerospace engineer. He transferred to ARO in 2014 as the Program Manager for Fluid Dynamics.

Current Scientific Objectives

1 | Understand and predict the dynamics of unsteady and separated flows, identifying critical parameters or "signatures" of incipient separation events for avoidance of boundary layer separation or generation of large aerodynamic forces and moments that, if successful, will improve Army vehicle and weapon system performance.

2 | Develop methods and tools enabling direct confrontation of nonlinearities inherent to the governing equations of fluid dynamics permitting global prediction capabilities and leveraging of those nonlinearities for novel effects that, if successful, will provide methods for improving future Army airborne system performance.

3 | Erect new frameworks for prediction of turbulent phenomena to overcome current methodologies that are largely limited to description that, if successful, will enable new models for turbulent behavior that permit the design of future Army leap-ahead technologies.

This success was made possible by:

Dr. Matthew Munson, Mechanical Sciences Branch

Dr. Frederick Gregory, Life Sciences Branch

Citations:

Mestre, H. *et al.* *Science* **367**, EAAX7171 (2020).

Hablitz, L. M. *et al.* *Nat. Commun.* **11**, 4411 (2020).

SUCCESS STORY

Clearing Your Head: The Mechanics of Glymphatic Waste Clearance

In response to a Multidisciplinary University Research Initiatives (MURI) topic call developed by Dr. Munson and Dr. Frederick Gregory (Program Manager for Neurophysiology of Cognition), a team at the University of Rochester and University of Wisconsin-Madison is combining neurophysiologists, sleep scientists, and mechanical engineers to describe and predict the brain's waste clearance system. Early successes have connected the glymphatic system with circadian rhythms and sleep states, as well as described the role of the system in stroke injuries and other acute trauma.

CHALLENGE

The brain clears metabolic waste through a mechanism known as the glymphatic system. Observations indicate the system is far more effective during sleep, but the actual governing mechanisms remain unexplained. The need to clear waste accumulated during waking hours—the cost of active cognition—is likely one reason that sleep is required.

The glymphatic system is a series of connected spaces surrounding the brain's blood vessels (termed perivascular spaces). The name is a combination of the lymphatic system (responsible for the body's waste clearance) and glial cells (which compose the structure elements of these spaces).

Several challenges to describing and predicting this system's dynamics exist, primarily because measurement inside the living brain is difficult. Additionally, any accurate description of the system depends on simultaneously answering many questions about the brain's activity, including:

Is the brain active or calm? Awake or asleep?

What is the composition of the fluid? How many and what kinds of waste products are present?

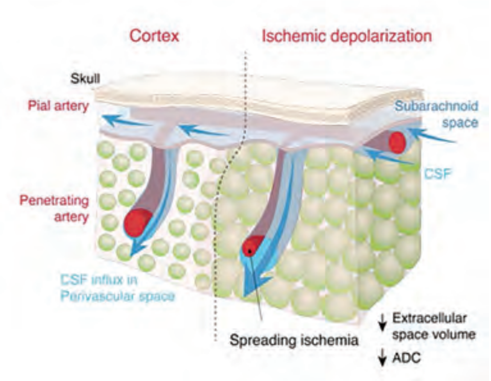


Figure 1: Spreading depolarizations propagate over the cortex, followed by spreading ischemia. The volume of the glymphatic network increases with vasoconstriction, driving flow into tissue and causing cellular swelling. Figure adapted from Mestre et al. (2020).

What is the condition of the flow? What are the pressures and velocities throughout the system?

What is the shape of the channels? Does this shape change over time, and if so, in response to what factors?

How does the brain's electrochemical activity influence fluid flow within the glymphatic system?

What are the most important factors that determine overall system performance?

How does the system's performance influence cognition?

Answers will allow for the description and prediction of system behaviors and hopefully lead to notions for deliberate regulation of system performance. Such control may allow improved cognitive performance in spite of chronic wakefulness by increasing waste clearance effectiveness. Additionally, a reduction in the probability of neurodegenerative disease development over the long term may be possible.

RESULT

In early 2020, researchers conducted an experiment to induce ischemic events (i.e., a stroke) in mouse brains to understand post-stroke swelling dynamics. Combining advanced imaging techniques, including magnetic resonance imaging (MRI), radiolabeled tracers, and multi-photon imaging, they showed that cerebrospinal fluid (CSF) surrounding the brain enters the tissue within minutes of a stroke event. The surprising observation was that perivascular spaces play an important role in accommodating these flows. The ischemic insult results in the loss of the brain's ability to maintain the cellular ionic balance required for control of cell water content. This depolarization event causes a constriction of the blood vessels, nearly doubling the perivascular space available to support glymphatic flow. Inflow of CSF via glymphatic pathways appears to be the primary driver for the initial swelling that happens after a stroke or other ischemic insult (such as traumatic brain injury) (Figure 1).

In another effort, observations of increased clearance performance during sleep led the team to question whether sleep timing relative to the day–night cycle had an impact on overall glymphatic effectiveness. Circadian rhythms, important for other sleep–wake related phenomena, may affect glymphatic flows. The team used advanced imaging methods in rodent models to determine the variation of the amount and direction of glymphatic flows across the day, independent of arousal state. They found (a) the glymphatic system exhibits diurnal variation, (b) variation persists in constant light (i.e., is not driven by light–dark cycles), (c) lymphatic drainage rhythms are opposite to glymphatic influx, and (d) elimination of specific water channels within glial cells important for enabling glymphatic function (aquaporin-4) eliminates the circadian effect. These results support the conclusion that glymphatic system performance is under circadian control. Multiple interconnected circadian interactions, including cortical neuronal activity, cardiovascular activity, and immune system functionality, are likely responsible for the overall promotion of circadian dependence on the glymphatic system (Figure 2).

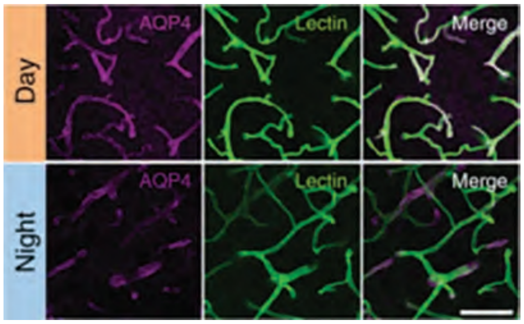


Figure 2: Representative ×63 magnification confocal images (day/night), showing increased polarization of aquaporin-4 around vascular structures, indicating greater influx of CSF into the brain during the day. Purple indicates water channels, green indicates vasculature, and white indicates the overlap between stains. White scale bar is 50 µm. Figure adapted from Hablitz et al. (2020).

ACTION

Drs. Munson and Gregory were able to secure funding from a 2020 Congressional Addition to support an investigation on the impact of chronic sleep restriction (CSR) to glymphatic function. This research will test whether a connection exists between the cognitive impairment associated with CSR and

ARL Competencies:

Biological and Biotechnology Sciences

Results

- Led to companion studies with MOMRP that are currently underway.
- Discovered the glymphatic system's role in ischemic injury outcomes.
- Discovered that the glymphatic system is subject to circadian regulation.

Anticipated Impact

Description and prediction of glymphatic system behavior is expected to enable future leap-ahead technologies such as sleep-efficiency improvement and mitigation of neurodegenerative diseases.

a persistent glymphatic waste clearance deficiency. CSR is prevalent across both military service members and the civilian population, so this effort will directly extend the original research and provide new opportunities to understand fundamental human performance.

These early scientific discoveries show promise for describing glymphatic system behavior and identifying possible therapies to mitigate the effects of ischemic events and non-optimal sleep patterns. Reduction of post-stroke brain swelling might be possible through glymphatic regulation, lessening secondary injuries and improving patient recovery outcomes. Deeper understanding of circadian-glymphatic regulation might lead to improved capability to construct appropriate sleep cycles for Soldiers and others suffering from duty-schedule-driven circadian misalignment.

Drs. Munson's and Gregory's efforts to promote these results to the broader Army and DoD communities have led to new efforts. The Defense Health Agency, in coordination with the Military Operational Medicine Research Program (MOMRP), has commissioned a study surveying the current state of understanding for glymphatic dynamics, specifically relative to sleep and human performance. Drs. Munson and Gregory have facilitated connections between the MURI team and the study lead, the Massachusetts Institute of Technology Lincoln Laboratory. As the MURI effort is at the forefront of this research, it will feature prominently in the study and provide significant influence over the direction of future efforts.

WAY AHEAD

These early accomplishments have already generated substantial interest both within the Army and beyond. As the research continues, Drs. Munson and Gregory will continue to capitalize on opportunities to connect Army and DoD researchers to this research area in order to accelerate the identification of new technology and therapeutic innovations, as well as communicate the implications for this research on analysis and mitigation of emerging operational threats.

This success was made possible by:

Dr. Matthew Munson, Mechanical Sciences Branch

SUCCESS STORY

The Knotty Problem of Vortex Dynamics

New insights from vortex dynamics afford intriguing opportunities to study turbulence under controlled conditions. In early 2018, Dr. Munson connected two researchers to tackle the tangle of turbulence, which has led to a new discovery that vortex reconnection cannot neglect the effects of viscosity. This discovery has implications for the accurate prediction of vortex dynamics and turbulent flows relevant to Army vehicle and munitions systems.

CHALLENGE

Turbulence is a perennially difficult problem. Very small changes in the initial or boundary conditions of a flow can generate perturbations that ultimately lead to large fluctuations. In addition, turbulence acts across a range of spatial and temporal scales in a given flow, with nonlinear interactions among those scales transferring energy between them in complex ways. Given this complexity, the specific details of a turbulent flow are incredibly difficult to predict. Similarly, experimental measurements of turbulent flows can be challenging, especially at the smallest scales, because the mere act of measuring such flows introduces disturbances that can fundamentally alter the dynamics!

ACTION

In 2018, Dr. William Irvine at the University of Chicago contacted Dr. Munson with an idea to use a novel vortex formation technique to experimentally study a confined "blob" of turbulence. Dr. Irvine envisioned a cubic chamber that would feature a vortex injection site on each corner. By carefully controlling both the shape of the nozzle and the amount of fluid injected through it, he would be able to adjust the strength of the vortex ring, along with the amount of "helicity" (a quantity describing the amount of twist and writhe on the ring). When the rings from each aperture arrived at the center of the tank, they would combine through a complicated process of connection and destruction, creating a spatially confined region of turbulent flow. Advanced quantitative flow visualization diagnostics can subsequently reveal the geometry and dynamics of this turbulent region (Figure 3).

Nearly simultaneously, Dr. Carlo Scalo from Purdue University contacted Dr. Munson with a new computational fluid dynamics formulation that showed promise to resolve very-small-scale turbulent features. A technique known as large eddy simulation (LES) has existed for quite some time; effectively it simulates flow features down to a certain size, with the dynamics of any small motions resolved through modeling instead of direct computation from first principles. Not only is the choice and the quality of the

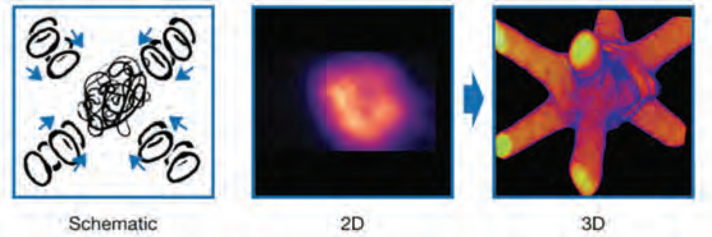


Figure 3: Colliding vortex rings create a controlled "blob" of confined turbulence for study. Courtesy of Dr. William Irvine.

model chosen to represent the small-scale dynamics important to the overall accuracy of the simulation, but an additional consequence of this methodology is that even large structures wind up subjected to artificially high levels of dissipation. Dr. Scalo's innovation was to construct a computational "sensor" that effectively measured the rate of local rotation (i.e., how fast a fluid "particle" was spinning) for each location in the simulation, which is then used to determine whether small-scale modeling should be employed at all. By running the small-scale modeling only where required, this coherent-vorticity-preserving LES formulation becomes capable of simultaneously avoiding the artificial dissipation at large scales while adequately resolving the smaller scales.

Dr. Munson immediately recognized the potential of Dr. Scalo's new LES method to simulate the same physics that Dr. Irvine was interested in investigating. Even as each investigator worked toward the development of their individual proposals, they both recognized the value of one another's capabilities and started collaborating informally. By the time each of their proposals was selected for award, the collaboration was solidly underway.

RESULT

To test the capability of the new LES formulation to capture small-scale vortex dynamics, Dr. Scalo started working on a problem that Dr. Irvine had previously studied: knotted trefoil vortices. In this problem, a 3D hydrofoil is accelerated in a water tank, leaving behind microbubbles trapped in the core of the vortex ring. The shape of the hydrofoil results in the creation of a continuously connected vortex ring that evolves in complex ways as the vortex interacts with itself, ultimately resulting in two separate vortex rings (Figure 4).

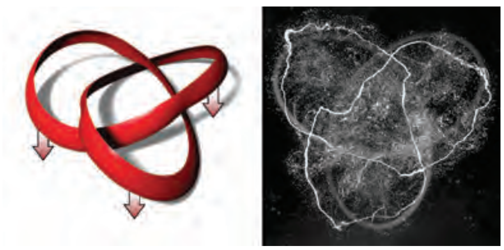


Figure 4: (Left) A 3D hydrofoil. (Right) A trefoil vortex knot in water imaged via light scattering from microbubbles. Courtesy of Dr. William Irvine.

One of the hopes was that Dr. Scalo's simulations would be able to reveal some of the small-scale dynamics associated with vortex breakdown, pinch-off, and reconnection, as these physical events are difficult to resolve via experiment. In combination with another innovation involving adaptive mesh refinement, Dr. Scalo was able to create high-fidelity simulations of the trefoil vortex behavior that showed fantastic agreement with Dr. Irvine's experiments (Figure 5).

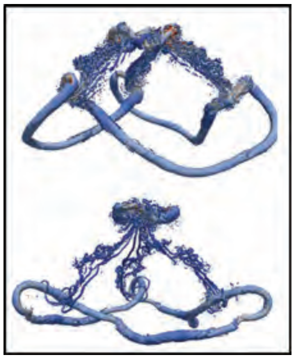


Figure 5: Coherent-vorticity-preserving LES of the late-stage development of a trefoil vortex. Courtesy of Dr. Carlo Scalo.

In addition, because the combination of innovations (coherent vorticity preservation and adaptive mesh refinement) focused computational power only where the most challenging physics was present, Dr. Scalo was able to run simulations with much stronger vortex dynamics than had previously been investigated. Doing so revealed a previously unknown result, namely, that fluid friction played an important role in vortex breakdown and reconnection. Previous vortex dynamics formulations had always assumed that this was an inviscid (friction free) process, but the simulations clearly demonstrate the error of this assumption.

WAY AHEAD

Dr. Scalo's innovations have the potential to simulate flows at an accuracy and efficiency level previously unobtainable, enabled by close collaboration with Dr. Irvine. This new formulation intelligently matches the level of simulation sophistication to the underlying flow physics in order to focus the computational horsepower exactly where required. ARL has engaged with Dr. Scalo to address some hypersonic aerodynamics investigations, and conversations are underway with the team that manages the DoD High-Performance Computing capability to determine the best way to scale this new capability to large-scale problems.

ARL Competencies:

Mechanical Sciences

Weapons Sciences

Results

- Led to a cooperative agreement with ARL to use computational methodologies to pursue hypersonic aerodynamics.
- Demonstrated a high-fidelity simulation of complex vortex dynamics.
- Discovered viscous effects for high-strength vortex dynamics.

Anticipated Impact

Advanced LES capability is expected to enable future leap-ahead technologies such as aerodynamic vehicle performance predictions and advanced munition designs.

PROPULSION AND ENERGETICS PROGRAM

Program Manager
Dr. Ralph Anthenien
Chief, Mechanical Sciences Branch

Dr. Anthenien completed his undergraduate studies at the University of California, Berkeley, receiving his B.S. in Mechanical Engineering in 1993. He received his Ph.D. from the University of California, Berkeley in Mechanical Engineering in 1998.

He came to ARO in 2006 as the Program Manager for Propulsion and Energetics.

Current Scientific Objectives

Overall, the program seeks to develop the ability to control chemical energy release rates in energetic materials and fuels via the understanding of phenomena governing initiation, burning, reaction, and extinction. This will be achieved through the following:

1. Determine the chemical and transport mechanisms that control ignition and initiation in high energy density systems, to include energetic materials, especially when subjected to thermal and mechanical insult, and heavy hydrocarbon fuels, especially at high pressure and low temperature, that, if successful, could lead to insensitive energetic materials and engine designs that allow for broad fuel flexibility.

2. Determine how to manipulate processes in materials and material interfaces to achieve control over reactions and reaction rates that, if successful, could lead to novel energetic materials with controllable energy release rates that could lead to significant increases in the energetic content of systems, increased power density, and tailorable effects for enhanced range or on targets.

This success was made possible by:

Dr. Ralph Anthenien, Mechanical Sciences Branch

SUCCESS STORY
Optical Characterization of Subsurface Reactions in Heterogeneous Materials

Work supported by ARO led to a demonstrated capability to measure subsurface fluorescence and Raman scattering of a molecular crystal embedded in an opaque heterogeneous sample. This represents a new ability to conduct subsurface, opaque material spectroscopy and will open new opportunity to studying the reaction chemistry of energetic materials.

CHALLENGE

Explosives and propellants are heterogeneous materials consisting of energetic molecular crystals (e.g., RDX and HMX) embedded in polymeric binders (e.g., elastomers and fluoropolymers). These typically consist of randomly oriented energetic crystals, with sizes ranging from sub-micrometer to hundreds of micrometers, embedded in a polymeric binder. These energetic materials can be initiated through a variety of stimuli, including thermal, mechanical, and electrical means. For example, as a shock wave travels through such a heterogeneous material, a variety of phenomena such as pore collapse, plastic deformation, micro-fractures, shear banding, and binder–crystal and crystal–crystal interface friction can take place. Each of these mechanisms can lead to localized heating with the temperature rise dependent upon the local rate of inelastic deformation versus the local heat dissipation. If sufficient heating occurs, these local hot-spots can lead to chemical reactions and energy release in the material. Most of these processes take place subsurface. Optical techniques such as Raman spectroscopy and Fourier transform infrared (FTIR) spectroscopy, which probe vibrational energy levels, combined with optical emission spectroscopy (OES) and optical absorption spectroscopy, which probe electronic energy levels, are some of the most common approaches to monitor chemical reactions. However, due to the heterogeneous nature of the materials of interest, a long-standing scientific issue has been to monitor chemical reactions that occur below the sample surface. The optical opaqueness, caused by optical scattering, makes it very difficult, if not impossible, to apply these spectroscopy techniques to optically monitor subsurface chemical reactions in these materials.

ACTION

Dr. Anthenien has challenged the diagnostics and energetics communities for several years to devise new methods for probing and monitoring subsurface chemical reactions in opaque materials. He worked closely with both these communities to communicate the challenges and worked through several ideas with many researchers via white papers and informal communications to explore potential efforts. Early in 2017, Professor Hergen Eilers of Washington State University proposed a method using optical phase conjugation to probe subsurface kinetics. An effort was awarded late in 2017.

RESULT

The approach seeks to overcome the challenge by combining a confocal microscope with isotropic focusing, which involves using two objectives (both the top and bottom of the sample), reducing the axial spot size to a near-diffraction limited value. This arrangement is challenging as the two microscope objectives need to be perfectly aligned and scattering can deteriorate the focal spot. The alignment challenge can be overcome by including optical phase conjugation (OPC) in the setup. OPC is a process that reverts the light to its origin. Here, light that is scattered through the sample and collected by the second objective is detected by a camera and a computer then calculates the OPC, generates it with the help of a spatial light modulator (SLM), and sends it back to the focal spot.

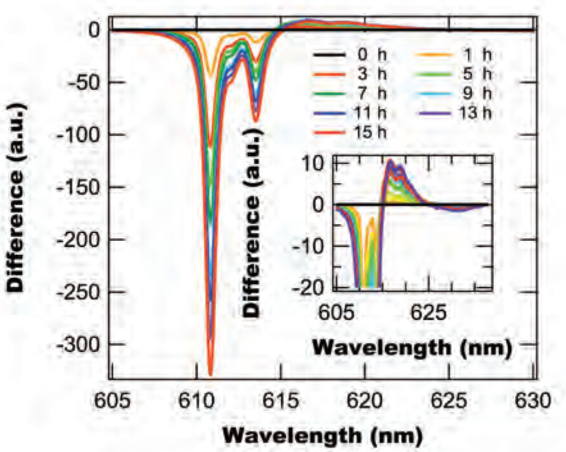


Figure 1: Optimized subsurface difference spectra during photodegradation. Insets show zoomed-in views of the spectra. Figure courtesy of Professor Hergen Eilers.

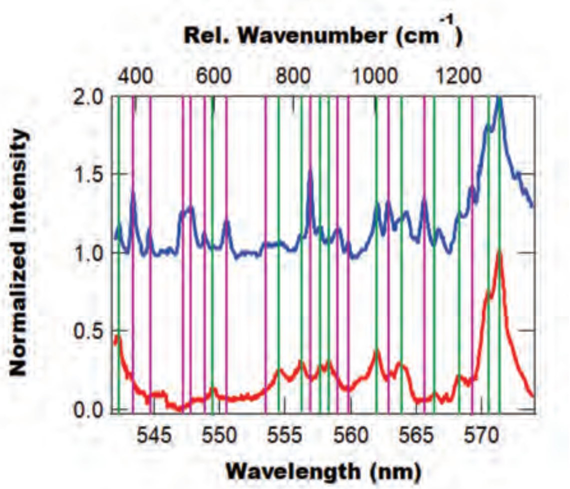


Figure 2: Raman spectra of polymer only (red curve) and sugar + polymer (blue curve). The green vertical lines mark polymer peaks and the purple vertical lines are sugar peaks. Figure courtesy of Professor Hergen Eilers.

The researchers then prepared several heterogeneous samples consisting of polymer matrices with embedded molecular crystals. They then inserted one or more fluorescent particles to serve as guide-stars. By monitoring and maximizing the fluorescence intensity using the spectrometer and charge-coupled device (CCD), they ensure the laser beam is focused onto the guide-star. Next, the phase of the forward scattered light, collected by the second objective, is measured and its phase conjugate is calculated and generated using an SLM. This light is sent back and focused onto the fluorescent particle. Finally, they optimize the laser-induced fluorescence (LIF) signal and perform Raman measurements on the sample to determine the overall quality and reproducibility of these measurements.

The researchers demonstrated the setup's ability to monitor subsurface chemical reactions by preparing a sample consisting of the guide-star material, europium- and dysprosium-doped yttrium molecular crystals (EYAD/DYAD), which have strong Raman scattering with well-defined peaks, dispersed into a hydroxyl-terminated polybutadiene (HTPB) polymer with sugar loaded at 50%. The researchers use wavefront-shaping-assisted bidirectional focusing to focus the beam onto the target particle inside a heterogeneous sample. This focus acts as both the probe beam and decay-inducing beam. Next, the Raman spectra were measured during photodegradation. This procedure is more complicated, as contributions from the LIF signal from the polymer and sugar are all observed in the spectral region where YAD is Raman active. To help deconvolve the spectra, different reference spectra were considered. They next considered the emission spectra measured in the Raman-active region from the heterogeneous sample during photodegradation as well as background

ARL Competencies:

Terminal Effects

Weapons Sciences

Results

- Discovered a new diagnostic method to probe chemical kinetics via Raman spectroscopy subsurface in a heterogeneous material.

Anticipated Impact

The new diagnostic technique will open the ability to gain new knowledge about the chemistry of energetic materials in pores and at grain interfaces. This, in turn, could lead to new inherently insensitive energetic materials with higher energy and power densities.

fluorescence from the heterogeneous material. Figure 1 shows the LIF spectra at different times during photodegradation as a difference spectra (i.e., spectra at time t minus the spectra at time 0). As the target particle degrades, the fluorescence changes are consistent with those measured in bulk EYAD. As a different way to visualize this decay, the researchers compared the normalized spectra at 0 and 20 h. It was found that the Raman peak locations remain the same at both times, with the primary difference being the addition of a significant broad background at time 0 h (the beginning of the experiment). As the sample is exposed to light, the broad background decreases and eventually the Raman peaks dominate. Given the very broad nature of the background, it is most likely due to fluorescence from the polymer. For reference, they also measured the Raman spectra of both a polymer sample and a sugar + polymer sample in order to determine which Raman peaks come from the sugar and which are from the polymer (Figure 2).

This work demonstrates the ability to probe Raman spectra from subsurface molecules in a heterogeneous material.

WAY AHEAD

Next, Washington State University researchers will finalize the alignment techniques of the system, implement a new bidirectional-feedback-assisted focusing technique, and compare the performance and implement and test the feasibility of an auto-alignment technique. Finally, they will test additional materials to further demonstrate the microscope's ability to characterize subsurface reactions. Dr. Anthenien will monitor the progress and coordinate with ARL WMRD researchers to form tighter collaborations that will allow transfer of the technique to Army laboratories.

This success was made possible by:

Dr. Ralph Anthenien, Mechanical Sciences Branch

SUCCESS STORY

Simultaneous Velocity, Temperature, and Formaldehyde Imaging to Study Ignition in High-Pressure Turbulent Jets

A diagnostic method has been developed to simultaneously probe velocity and temperature in evolving mixtures at engine-relevant pressures and temperatures. This provides a method to study turbulent fuel jets in compression-ignition engines.

CHALLENGE

The complex coupling of turbulence and chemistry is difficult to probe especially at temperatures and pressures relevant to engine conditions. This has left the mechanism of ignition in high-pressure turbulent fuel jets not fully understood. Several numerical simulations have led to complex conceptual models for high-pressure jet ignition at diesel-engine-relevant conditions. These remain, unfortunately, largely unvalidated due to the lack of experimental measurements. Model validation and development of a deeper understanding of the ignition mechanism of heavy hydrocarbon fuels at high pressure and low (800 K) temperature require simultaneous measurements of velocity, temperature, and chemical species fields. Preliminary work using aerosol phosphor thermometry (APT) coupled with particle image velocimetry (PIV) to make high-precision temperature measurements simultaneously with velocity measurements has shown promise to achieve these goals.

Recent work funded by ARO through a Short-Term Innovative Research (STIR) grant has shown the promise of APT to make high-precision temperature measurements at temperatures relevant for high-pressure jet ignition. Measurements of temperature using APT are readily coupled with PIV using seeded particles to simultaneously measure the velocity and temperature fields.

ACTION

In 2009, Dr. Anthenien developed a Small Business Technology Transfer (STTR) topic that called for a capability to develop a simultaneous particle image velocimetry thermometry (PIVT) system for use in turbulent reacting systems. University of Wisconsin researcher Professor David Rothamer collaborated on the successful STTR Phase I and Phase II contracts. Initial work showed promise at moderate temperatures (up to 800 K) and ambient pressures. The low temperature allowed tracing of the reacting flow field up to the point of ignition but did not allow for tracking through the reacting flame. Follow-on work with Professor David Rothamer at the University of Wisconsin, funded under a STIR grant in 2018, demonstrated a path to improve the accuracy of this approach. A Single Investigator grant was awarded in 2019 to further advance the PIVT method up to 1300 K and at elevated pressures up to 100 bar. The proposed work further combined the PIVT method with formaldehyde planar laser-induced fluorescence (PLIF) to allow for monitoring of this early ignition precursor.

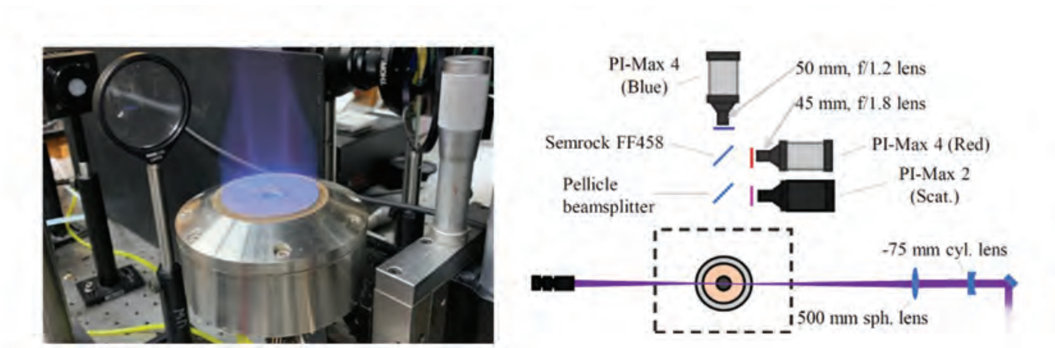


Figure 3: Experimental setup used for APT imaging of Ce,Pr:LuAG, Ce:$GdPO_4$, and Ce: $Ca_3Sc_2Si_3O_{12}$: (left) image of the jet with the concentric flame flat and (right) schematic showing the layout of the laser sheet and sheet-forming optics and cameras and used for collecting Mie scattering and luminescence signals. Figure courtesy of Professor David Rothamer.

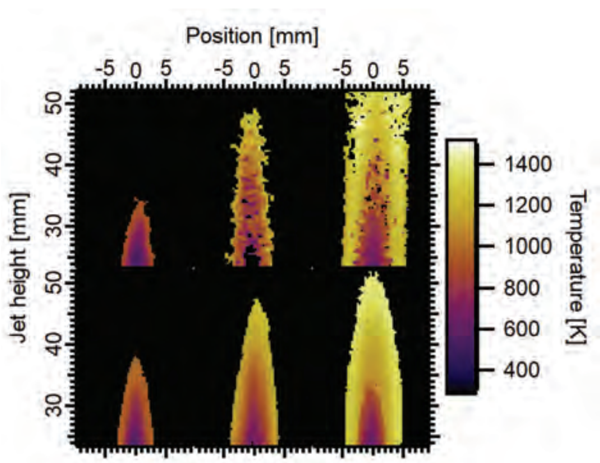


Figure 4: Single-shot (top row) and median (bottom row) temperature images from Ce,Pr:LuAG (left), Ce:$GdPO_4$ (middle), and Ce: $Ca_3Sc_2Si_3O_{12}$ (right) phosphors. Single-shot seeding densities (at the jet center, 23 mm above burner) are 650 mm^{-3} (Ce,Pr:LuAG), 60 mm^{-3} (Ce:$GdPO_4$), and 130 mm^{-3}(Ce:CSSO). Figure courtesy of Professor David Rothamer.

RESULT

Researchers at the University of Wisconsin have studied and developed three different three phosphors (Ce,Pr:LuAG, Ce:$GdPO_4$, and Ce:$Ca_3Sc_2Si_3O_{12}$) for the coating seed used in the PIVT systems at combustion-relevant temperatures. To first demonstrate the new temperature range of the phosphors, they imaged the flow in a jet mixing with a concentric flat flame, as in Figure 3. Single-shot precision of 20 K or better was demonstrated over the temperature range from 500 to 1300 K, demonstrating the capability to meet previously unachieved precision. The researchers also achieved single-shot temperature imaging at temperatures up to 1400 K, approximately 500 K higher than previous single-shot APT measurements. Exemplar results of the temperature imaging information are shown in Figure 4.

WAY AHEAD

University of Wisconsin researchers have further applied scattering-reference APT (SRAPT) to the commonly used phosphor europium-doped barium magnesium aluminate (BAM:Eu). Results demonstrate the ability to expand the temperature imaging range to higher temperature using SRAPT compared to the commonly used spectral intensity ratio method. This gives a path to still higher temperature ranges for the PIVT method. Dr. Anthenien is working with ARL researchers to transition these techniques to allow for use of the method in Army laboratories to validate and improve combustion models for engines in vehicles and aircraft.

ARL Competencies:

Energy Sciences

Results

- Discovered a new diagnostic method to probe temperature, velocity, and chemical species simultaneously to elucidate combustion mechanisms in turbulent reacting flows.

Anticipated Impact

Previously unattainable validating experimental data will be available at engine-relevant temperatures and pressures. This will open the way to new combustion and engine design models.

SOLID MECHANICS PROGRAM

Program Manager Dr. Denise Ford

Dr. Ford completed her undergraduate studies at the University of Wisconsin-Madison, receiving her B.S. in Chemical Engineering in 2007. She trained as an engineer at the Fermi National Accelerator Laboratory and Northwestern University, receiving her Ph.D. in Chemical Engineering 2013.

She came to ARO in 2019 as the Program Manager for the Solid Mechanics.

Current Scientific Objectives

1 | Uncover the physical processes responsible for deformation, damage initiation and propagation, and failure of material systems that, if successful, could lead to the creation of ultra-resilient, lightweight, and durable Soldier and system protections.

2 | Develop computationally efficient, robust, and predictive models that, if successful, could substantially reduce the time and cost required to develop new material systems.

This success was made possible by:

Dr. Denise Ford, Mechanical Sciences Branch

Dr. Ralph Anthenien, Mechanical Sciences Branch

Citations:

Chandler, D. L. "Machine-Learning Tool Could Help Develop Tougher Materials," *MIT News*. (2020).

SUCCESS STORY

A Nature-Inspired Library for the Design of Lightweight Impact-Resistant Materials

A library of nature-inspired structures for material design is being developed through new methods utilizing artificial intelligence (AI) to predict the physical and mechanical properties of and fracture processes in materials.

CHALLENGE

Nature offers a wealth of inspiration for high-performing systems that combine strength, stiffness, toughness, and low weight; however, researchers have had a difficult time mimicking these properties in synthetic systems. In particular, the complex 3D shapes and hierarchical structures found in nature create a vast design space, multiscale challenges to property evaluation and prediction, and challenges to correlating structural features to properties and performance.

ACTION

Program managers at ARO realized that AI-based methods could drastically speed up material property predictions, if properly trained, and could be applied to extremely complicated systems. Recognizing Professor Markus Buehler at the Massachusetts Institute of Technology as a leader in the field, Dr. Ralph Anthenien, former acting Program Manager for Solid Mechanics, encouraged him to submit a proposal to create an analysis technique for and property database of triply periodic minimal surface (TPMS) structures, a family of structures found in lightweight, thermally conserving, impact-shielding butterfly and beetle wings. Some examples of TPMS are shown in Figure 1. To achieve these goals, theory, computation, and experiment

"Lab tests or even detailed computer simulations to determine their exact properties, such as toughness, can take hours, days, or more for each variation. Now, a new artificial intelligence-based approach developed at MIT could reduce that to a matter of milliseconds."

– From Chandler (2020)

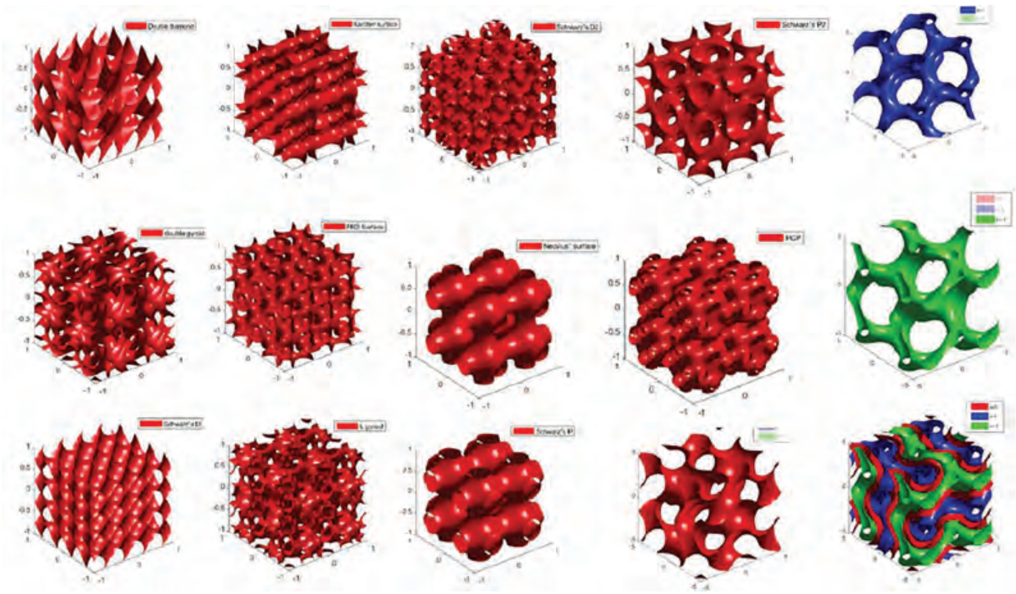


Figure 1: Examples of triply periodic minimal structures in the library. Figure courtesy of Professor Markus Buehler.

would be required. Therefore, the proposal was awarded as a cooperative agreement in 2019 to leverage collaborations and specialized equipment available at the Institute for Soldier Nanotechnologies (ISN), a DoD University Affiliated Research Center (UARC).

RESULT

Professor Buehler completed studies on the deformation and fracture of three different surface topologies with 3D graphene foams, which provided a systematic understanding of the relation between TPMS topologies and their mechanical properties, including the failure mechanisms of graphene foams. He also developed a design approach for optimizing the toughness of nanocomposite materials using AI, which consists of a machine learning predictor combined with an AI-improved genetic algorithm, facilitated by a deep convolutional neural network that is trained with a dataset of hundreds of thousands of combinations of soft and brittle materials originating from a finite element analysis. The solutions generated by the AI model require dramatically less computational time and fewer resources compared to brute-force searching methods. Professor Buehler also developed a method to predict stress and strain fields in complex scenarios under varied loading conditions using a generative adversarial neural network for architected gyroid and other porous materials, a semi-supervised approach to architected materials design using graph neural networks, and a method using deep learning to predict fracture patterns in crystalline solids, which was featured in an *MIT News* article (Chandler, 2020). He has also developed and gave a professional short course on AI methods for materials design, which was attended by ARL and other DoD scientists.

WAY AHEAD

Professor Buehler will continue to investigate the structure–function relationship of structures within the family of TPMS geometries in effort to develop a comprehensive solid mechanics theory of the behavior of TPMSs. He also plans to develop a data-driven machine learning algorithm to optimize the design across different topologies. Finally, he will build prototypes of structures for experimental tests at the ISN. If successful, these advances will contribute to a new set of tools to design and predict the performance of new strong and lightweight structures.

ARL Competencies:

Terminal Effects

Weapons Sciences

Results

- Developed new AI methods for predicting the mechanical properties of and fracture processes in a library of nature-inspired materials.
- Trained DoD scientists in AI methods for materials design through a professional short course.
- Collaborated with ARL scientists through the ISN at MIT.

Anticipated Impact

The methods and materials database developed in this work are expected to enable the nature-inspired design of multifunctional materials for Army structural and protection systems.

This success was made possible by:

Dr. Denise Ford, Mechanical Sciences Branch

Dr. Ralph Anthenien, Mechanical Sciences Branch

SUCCESS STORY

Novel Optical Technique for Impact-Induced Damage Evolution in High-Strength Low-Toughness Materials

This ARO initiative resulted in a new understanding of dynamic crack growth across an interface in layered transparencies and a novel optical technique for studying such phenomena.

CHALLENGE

Damage evolution is difficult to visualize and quantify in high-strength, low-toughness materials, such as the transparent glasses used for windows in armored vehicles, due to high crack growth speed. Yet understanding how damage propagates in a material system is critical to enhancing a system's performance. In addition to impact resistance, weight and cost are important considerations. Layering transparent materials may mitigate dynamic damage propagation as well as reduce weight and cost; however, crack propagation and stress attenuation across the interfaces as well as the effect of the adhesive between layers are poorly understood.

ACTION

Through the support of the Solid Mechanics Program, Professor Hareesh Tippur of Auburn University has been developing a full-field, vision-based, non-contact technique capable of measuring stress gradients and stresses. Professor Tippur developed the original digital gradient sensing (DGS) technique, via a Single Investigator (SI) grant in 2008, which is capable of measuring two orthogonal stress gradients in transparent solids and surface slopes in opaque reflective solids. ARO program managers realized that this technique could be adapted and applied to layered transparencies and awarded Professor Tippur another SI grant for this work in 2016. The setup was adapted and then used to answer questions such as the following: Would a growing crack arrest at the interface, penetrate the interface, and enter the subsequent layer as a single or multiple branched cracks? Can these phenomena be controlled by altering interfacial strength, elastic/inelastic characteristics of interface materials, layer thickness, location of the interface, and/or uniform versus functionally graded layering? How do interfaces alter stress wave histories in layered structures and, in turn, influence the evolution of stresses at the impact location?

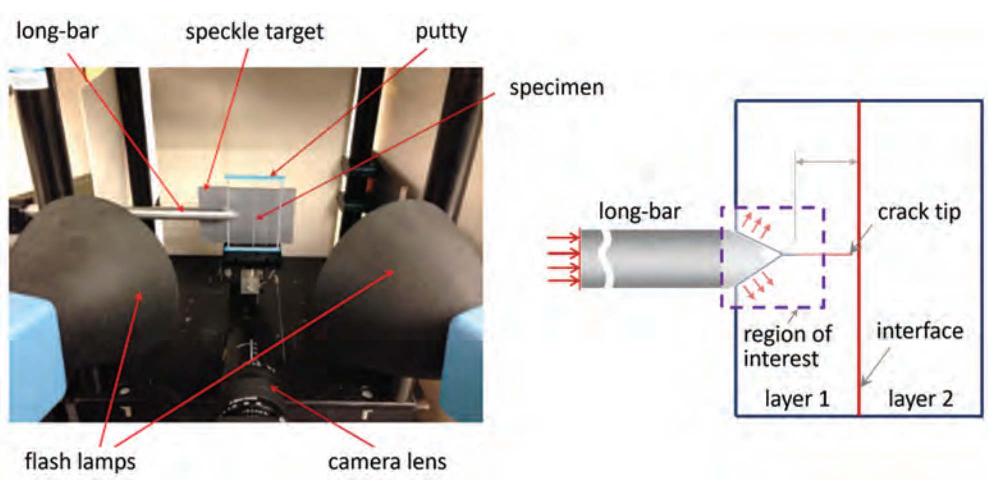


Figure 2: DGS technique adapted to study layered transparent materials. Figure courtesy of Professor Hareesh Tippur.

As the work evolved, the need for an enhanced light source, illumination system, and camera lens arose, which were funded by a Research Instrumentation grant in 2017. Throughout the project, Professor Tippur has interacted extensively with ARL WMRD scientists by sharing data and provided a four-day training to ARL WMRD scientist Dr. Chris Meredith. As the grant was coming to a close in late 2019, Dr. Ford and ARL WMRD scientist Dr. Sikhanda Satapathy realized that the technique could be further adapted and extended to study opaque armor ceramics, such as alumina and silicon carbide. Dr. Ford is currently working with Professor Tippur on the next steps to continue knowledge development in this area.

RESULT

Professor Tippur has adapted his DGS technique, shown in Figure 2, to study dynamic crack propagation across interfaces in layered transparent materials. In transmission mode, the setup

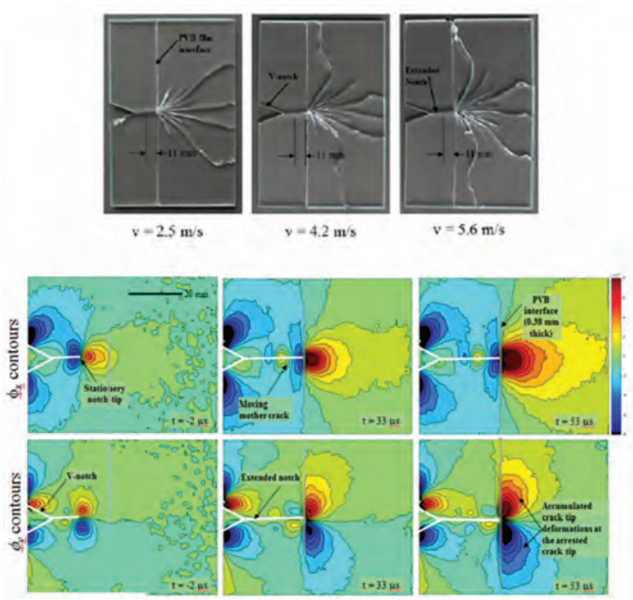


Figure 3: Fracture patterns for an impactor driving a mode-I crack through a soda-lime glass bilayer joined with a PVB film at three different striker velocities (top) and stresses prior to crack branching captured using DGS for the 2.5-m/s impact (bottom). Figure courtesy of Professor Hareesh Tippur.

consists of a planar surface target with random pattern/speckles, a digital camera, incoherent broad-spectrum illumination lamps, and the solid specimen. The random speckle pattern on the target is first recorded by the camera in the undeformed state of the specimen to obtain a reference image. Upon loading, the non-uniform stresses due to the imposed loads alter the refractive index of the specimen locally. Additionally, the Poisson effect causes local non-uniform thickness changes. A combination of these makes light rays deviate from their original path as they propagate through the stressed specimen. The random pattern on the target is again recorded through the specimen in the deformed state. The local deviations of light rays between the two exposures are quantified by performing 2D digital image correlation of the two images to quantify shifts in the speckle clusters. To subject the specimen to dynamic impact, a V-notch is cut into layer 1 of a bilayer specimen and placed in contact with a tapered-tip long-bar. The long-bar is then impacted by a striker propelled by a gas-gun to initiate the crack. Some results of Professor Tippur's studies are shown in Figure 3. Here, two soda-lime glass strips are joined using polyvinyl butyral (PVB) film to make a glass bilayer specimen with a strong ductile interface. The results for an impactor driving a mode-I crack at three different striker velocities are shown. When the crack reaches the interface, it stops and accumulates energy before producing "palm-tree" fracture patterns with an increasing number of daughter cracks with increasing impact velocity. The angular deflection of light rays, which are proportional to the two in-plane spatial gradients of stresses, prior to branching are captured using DGS and an example for 2.5-m/s impact is shown. The first column represents pre-initiation phase, the second and third represent arrested crack in the PVB layer.

WAY AHEAD

Many open questions remain about dynamic crack propagation during high-velocity impact. Professor Tippur will continue to adapt the DGS technique to study other Army-relevant systems and continue collaborations with ARL scientists, which include sharing of data and technique trainings. The transfer of this technique to ARL WMRD has the potential to enhance understanding and design of armor systems.

ARL Competencies:

Sciences of Extreme Materials

Terminal Effects

Results

- Filed an invention disclosure for the DGC technique.
- Trained an ARL WMRD scientist on the use of the DGS technique.
- Shared results and technique training with ARL WMRD scientists.

Anticipated Impact

The DGS technique and newly obtained physics on dynamic crack interaction with interfaces are expected to accelerate the development of enhanced protection systems.

Human Dimension Program

Program Manager
Dr. Frederick D. Gregory

Dr. Gregory completed his undergraduate studies at Morehouse College, receiving his B.S. in Biology in 1999. He trained as a neurobiologist at the University of California, Los Angeles, receiving his Ph.D. in Neurobiology in 2006.

He came to ARO in 2012 as the Program Manager for what was then called the Neurophysiology and Cognitive Neuroscience Program and then took on the additional role of International Program Manager for Human Dimension in 2016.

CURRENT SCIENTIFIC OBJECTIVES

1 | Develop a comprehensive understanding of the neural and physiological mechanisms that dictate the interface between brain and body that, if successful, will lead to materiel solutions that address the mind–body interface at novel nodes for maintaining cognitive and physical performance.

2 | Develop new theories to understand the dynamic interrelationships between individual/group cognition, decision-making, and the role these influences play on interactions in large and small social systems that, if successful, will lead to the capability to predict social-level phenomena with greater accuracy.

This success was made possible by:

Dr. Frederick Gregory,
International Division

SUCCESS STORY
The Ear as a Route to Augmented Soldier Performance and Machine Integration

ARO-funded research has led to the development of a novel prototype wearable device that measures and identifies brain and body biophysiological signatures in one form factor that has transitioned into a device development collaboration with ARL and DEVCOM AC. This new device paves the way for in-ear biophysiology as a novel platform wearable solution for nonintrusive Soldier monitoring.

CHALLENGE

The need to act quickly and decisively in battle can mean the difference between life and death. Physical stress, fatigue, cognitive load, and complex environments affect split-second and less consequential decision-making in ways that can lead to failures in fulfilling mission-critical tasks. As a result, there is intense interest in developing tools to ensure Soldiers maintain peak cognitive resilience under all physical conditions in order to instill cognitive dominance throughout a mission.

Brain–computer interfaces (BCIs) have emerged as the next frontier of neural engineering approaches to drive enhanced individual and squad-level performance. So far, however, it has not been possible to monitor brain function in real-world scenarios that are operationally relevant to the Soldier. Electroencephalography (EEG) measures of brain activity and physical performance metrics (like electrocardiograms (ECG) for measuring cardiac function) are traditionally confined to medical settings and laboratories. Monitoring brain electrical activity requires wearing caps or nettings with sensors; these are wired and uncomfortable, they interfere with task performance, and the recordings are sensitive to contamination from movement that interferes with the signal. The neurotechnology industry is beginning to emerge with another set of wearable sensors that allow some forms of non-laboratory-based measures of brain activity. Therefore, enabling BCIs outside the laboratory represents a technical and scientific opportunity to move the field forward.

ARO initiated actions, beginning in 2014, to enable combined neural and physiological measures with the vision of driving real-time, seamless BCIs that gather Soldiers' biosignals and rapidly adapt to current physical and mental states. For example, when detecting Soldier fatigue, a system display screen might offer resources or options to reduce cognitive load or support decision-making.

This vision motivated program managers to lay the groundwork for an international collaboration that has resulted in technology transfer and research collaboration with the Army that could lead to numerous opportunities to enhance individual Soldier performance.

ACTION

Dr. Gregory and now-retired ARO Data Fusion Program Manager, Dr. Liyi Dai, discussed potential opportunities to accelerate the creation of next-generation BCIs at the final review meeting of the 2008 ARO Multidisciplinary University Research Initiative (MURI) program on Brain Network Analysis and Modeling for Communication and Orientation. This project's conclusions and outcomes pointed out that the state of the art in noninvasive neurophysiological measures would not enable deployment of future BCIs that exceeded capabilities beyond being able to move a cursor on a screen with brain signals, for example, or elicit a coarse motor command to a wheelchair or prosthetic limb. However, the project's outcomes also pointed to an opportunity that led Drs. Gregory and Dai on a new path to enable future advances for the Warfighter. Dr. Gregory's Neurophysiology of Cognition Program had already begun to focus toward the idea that future BCIs should take advantage of the fact that the brain and body are intricately connected. In this view, he and Dr. Dai wanted to take lessons learned from their concluding MURI project and steer the field toward a more holistic view, developing a data fusion strategy that takes advantage of brain and body signals as a vital stream of information about cognitive and physical state for future BCI.

Just prior to the MURI project's completion, the Obama administration launched the White House Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative with the goal of supporting the development and application of innovative brain technologies to create a revolution in our understanding as well as ability to treat brain disorders. This action triggered other nations to make similar bold investments in neuroscience research, like the European Union, which committed an investment of €1B to advance European neuroscience, computing, and brain-related medicine. With this widespread interest sweeping the globe, Drs. Gregory and Dai set out to ensure that the Army was participating in this push to understand the brain as well as support the transition of outcomes to benefit Soldiers. As a result, they formulated a new MURI topic to drive multidisciplinary research that would enable a novel computational framework for modeling and analysis of multimodal brain data.

This new MURI topic call focused on the incorporation of brain and body signals as input to a novel closed-loop BCI framework, providing real-time feedback and awareness of user state. Unlike most MURI topics that only support a team of U.S. researchers, this topic caught the attention of the United Kingdom's Ministry of Defence as they had agreed to partner with the DoD and co-fund select MURI topics. Drs. Gregory and Dai's topic made a lot of sense, given Europe's interest in leading a revolution in neuroscience. As one of the four topics that received this honor of U.S.-UK bilateral investment, the U.S. members of the MURI team were able to take advantage of a new transatlantic collaboration to address the topic's lofty goals. In late 2016, Dr. Maryam Shanechi from University of Southern California and Professor Yiannis Demiris at Imperial College London began to co-lead their international team of MURI co-investigators to develop new methodologies for modeling multimodal physiological and neural activity underlying multisensory processing and decision-making.

At the kickoff for this MURI in 2016, Dr. Gregory had just moved to London to initiate the international Human Dimension Program. While in London, he visited Professor Danilo Mandic at Imperial College London, one of the U.S.-UK MURI team co-investigators. Professor Mandic had developed a prototype in-ear biophysiological sensor, which includes EEG, to measure human mental and physiological state (Figure 1) in a simulated driving task for the project. Dr. Gregory realized the unique technical and scientific opportunity enabled by the novel ear-based sensor platform and shared this message with Army scientists.

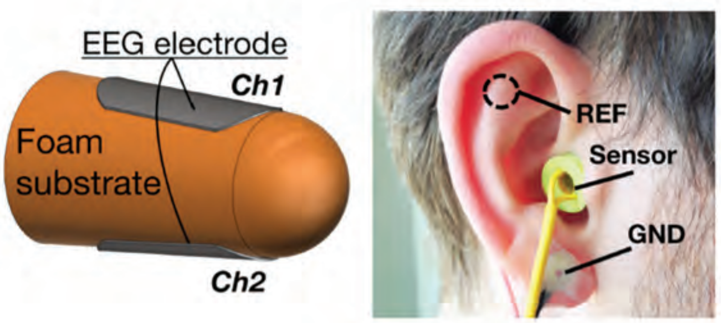


Figure 1: The EEG-only version of the prototype in-ear sensor. (Left) Depiction of a wearable in-ear sensor made from a foam substrate and containing two flexible electrodes (Ch1 and Ch2); additional sensor modalities can be incorporated. (Right) Placement of the prototype in-ear sensor. Courtesy of Professor Danilo Mandic.

ARL Competencies:

Humans in Complex Systems

Results

- Led to a framework for the design of closed-loop adaptive algorithms for a new class of brain–computer communication.
- Enabled collaboration with Army scientists that is leading to device development, test, and evaluation of a prototype device generated by an ARO MURI.

Anticipated Impact

As the MURI program comes to a close in 2022, it is anticipated that the research outcomes will lead to prototype BCIs for enhanced decision-making under heavy mental load, greater situational awareness, and object detection. It is hoped that these outcomes will provide a foundation for a paradigm shift in Soldier–armament integration and augmented Soldier performance.

Wearable sensors such as Fitbits and watches are ubiquitous in the wellness industry, but can only log steps, heart rate, and pulse. No available solution exists that also measures brain activity. On a visit to DEVCOM AC, the program manager met with scientists in the Tactical Behavior Research Laboratory that pointed to a specific need for Soldier cognitive and physiological assessment in tactical training environments outside the lab. Dr. Gregory introduced DEVCOM AC and ARL scientists to Professor Mandic in late 2018 and they immediately began to seek an opportunity to support collaboration.

RESULT

In laboratory experiments for the U.S.-UK MURI project, Professor Mandic's team at Imperial College London has proven the concept of a miniature and portable in-ear signal acquisition device capable of recording signals, providing direct information about brain, heart, and respiratory function (Figure 2).

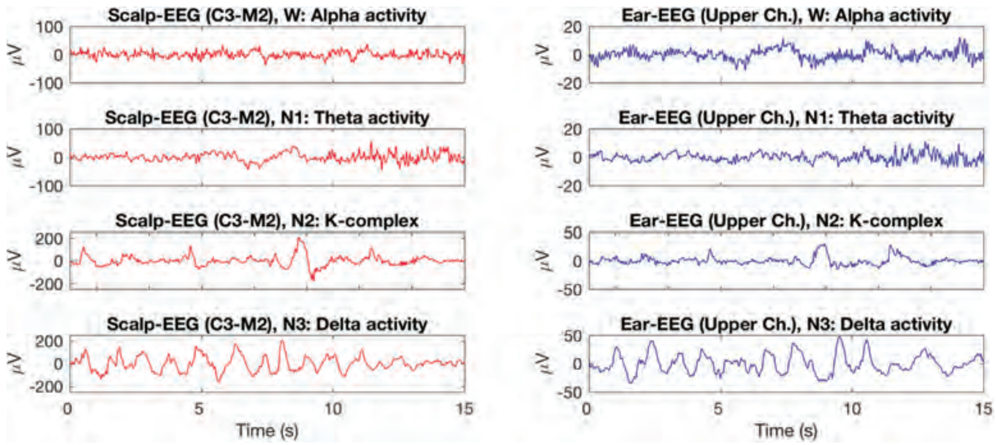


Figure 2: EEG recordings from a single participant in different sleep stages, demonstrating a side-by-side comparison with traditional scalp recordings (red: the on-scalp C3-M2 channel; blue: in-ear upper channel). Courtesy of Professor Danilo Mandic.

Nevertheless, because of its unusual location, this prototype device had lingering questions to address before it could be used for Soldier assessment, such as signal fidelity and potential susceptibility to motion artifacts. To address these questions requires a rigorous longer-term study, both in terms of the underlying sensing/electronics platform and novel signal conditioning/feature extraction solutions. Thus, Professor Mandic has formed a new alliance with DEVCOM AC and ARL scientists to tackle further development, testing, and evaluation. This new Army-Imperial College London team successfully competed for additional funding to enable further development of the prototype device in order to increase the technology readiness level and support future testing in Army tactical training and research environments.

WAY AHEAD

This joint effort, which begins in FY21, has the dual benefit of laying the foundation for delivery of a fieldable solution that would meet the size, weight, and power requirements for the Warfighter as well as enabling a better research tool that will directly benefit the MURI academic team's basic research effort. The result of this effort is intended to lead to a fieldable in-ear device, equipped with biosensing electrodes and coupled with robust signal processing, which would offer a unique way to deliver a high-quality BCI in a combat that can extract information about the levels of fatigue, stress, or engagement.

I D International Division

Innovations in Materials

Program Manager
Dr. James Harvey

Dr. Harvey completed his undergraduate studies at the United States Military Academy, receiving his B.S. in Engineering in 1964. He received an M.A. in Physics at Dartmouth College in 1972. He trained as a physicist at Lawrence Livermore National Laboratory, receiving his Ph.D. in Applied Science from the University of California, Davis in 1991.

He came to ARO in 1994 as the Program Manager for the Electromagnetics Program.

CURRENT SCIENTIFIC OBJECTIVES

1| Discover new opportunities for advances in materials science from the international basic research community within the overall vision of the ARO Materials Science Branch that, if successful, will enhance the materials science capabilities in the U.S. basic research community to support new U.S. military capabilities.

2| Focus on unique strategies and designs for optimizing materials with uncharacteristic or unexpected properties, architectures, and compositions, and explore new processing methodologies and unique instrumentation capabilities that, if successful, will enable lighter armor, lighter aircraft, and ground vehicles; more capable, efficient, and secure electronics systems; more-effective use of power; lower life cycle costs of military systems; and materials performance in extreme conditions.

SUCCESS STORY

Bringing Consistency to Laser Powder Bed Fusion Processing of Metal Alloys

A two-principal investigator collaborative project was started in 2018, leveraging unique capabilities in EMPA (Federal Swiss Laboratories for Materials Science and Technology) and Northwestern University (NWU; United States), to develop a better understanding of the physical and chemical dynamics of the selective laser melting (SLM) process for superalloys. The project achieved significant interim successes in establishing the roles of crack generation, the role of oxide dispersion and precipitation strengthening, and the entirely unexpected pathologies in the use of the traditional oxides employed.

CHALLENGE

Additive manufacturing (AM) has received major attention from the materials community because of its potential for extremely rapid fabrication of a wide range of shapes. SLM, also known as laser powder bed fusion (LPBF), has become the AM method of choice because it provides greater control of the melting process than other methods, can fabricate a wider variety of complex shapes, and provides greater control of the layered process (Figure 1). A very wide range of metal superalloys have been fabricated with extremely high operating temperatures. These alloy systems have extremely complex compositions and microstructure. For example Inconel, a nickel (Ni)-based alloy used in gas turbine blades, is composed of various parts of Ni, iron, molybdenum, chromium (Cr), niobium, cobalt, manganese, aluminum (Al), titanium (Ti), silicon, carbon, sulfur, and phosphorus, each of which react differently with competing effects within the microstructure. In the past, each of these complex alloy compositions has been studied at the microscale, with little general understanding resulting that could apply to more than one composition.

ACTION

In 2017 Drs. Michael Bakas, Julie Fife, and Chakrapani Varanasi of ARO were seeking to develop small co-funded efforts between the Materials Science Branch and the International Program that would develop collaborations between U.S. university researchers and international researchers where there

This success was made possible by:

Dr. Michael Bakas,
Materials Science Branch

Dr. Julie Fife, International Division

Dr. Chakrapani Varanasi,
Materials Science Branch

Dr. James Harvey,
International Division

Figure 1: SLM process. Courtesy of Professors Dunand and Leinenbach.

were significant unique complementary skills and ideas that would make major advances in materials science of interest to the DoD. Dr. Fife recognized the emerging collaboration between Professor David Dunand (NWU in the United States) and Professor Christian Leinenbach (EMPA in Switzerland). Professor Dunand was an expert on the properties of the microstructure of alloys resulting from SLM and a pioneer on the use of atom probe tomography (APT). Professor Leinenbach was an expert on AM processes and had recently developed a novel oxide dispersion strengthened (ODS) alloy, TiAl, with the breakthrough result that it could be melted and rapidly solidified into complex shapes while maintaining the oxide dispersoids within the grains of the alloy. Keeping the oxide dispersoids within the grains was critical for strengthening the alloy. At a conference in Italy, Dr. Fife engaged the two professors and encouraged them to apply to the Innovations in Materials Program.

Engagements with Dr. Bakas and the two professors resulted in a grant with the approach to focus on a simplified model Ni alloy: Ni, Cr, Al, Ti, with yttrium oxide (Y_2O_3) for oxide dispersion strengthening to identify the fundamental interactions of the constituents and their effects on microstructure, and its effect on macroscopic material properties. An in-depth multiscale study was proposed from macroscale to atomic-level analysis using transmission electron microscopy (TEM), electron backscatter diffraction (EBSD), high angle annular dark field-scanning electron microscopy (HAADF-STEM), and APT.

RESULT

This is believed to be the first in-depth LPBF study of an industrial alloy-inspired model alloy with characterization of grain structure down to local atomic chemistry and correlated with macroscopic properties. A number of lessons have already been demonstrated that will have a major impact on the entire field of AM. The study demonstrated that solidification cracking and liquation cracking can be eliminated and that the dominant cracking mechanism is ductility-dip cracking along high angle grain boundaries. A critical first demonstration is that solid solution strengthening, precipitation strengthening, and oxide dispersion strengthening can coexist and complement each other with the right parameter control. Solid solution strengthening occurs when an atom with a size different from the matrix atoms occupies a site in the crystal lattice of an alloy, creating a highly local distortion in the lattice, which inhibits sliding between lattice planes. Precipitation strengthening occurs when fine particles of an impurity phase, in this case $Ni_3(Al,Ti)$, impede the movement of dislocations or defects in the crystal lattice. Oxide dispersion strengthening occurs when oxide particles also form within the grains and impede the movement of dislocations as well as change the grain growth (Figures 2 and 3).

Figure 2: TEM and STEM micrograph of Ni superalloy microstructure. Courtesy of Professors Dunand and Leinenbach.

Figure 2 (top) shows the grain structure of a Ni-Cr-Al-Ti alloy. The different colors designate grains, which can differ by crystal orientation and alloy phase. The elongated grains running generally parallel promote the sliding of the grains with

This collaborative project demonstrates the value of the ARO International Division in bringing unique international expertise to bear on U.S. Army science issues and enhancing the capabilities within the U.S. scientific community available to work on Army programs

respect to each other, "creep," which decreases macroscopic strength. The bottom part shows the increased texture in the grains resulting from the addition of the oxide Y_2O_3, which is conventionally used in the fabrication of superalloys. The HAADF micrograph in Figure 3 highlights the local grain boundaries, which are superimposed on the APT picture in middle part. A major surprise is that the Y_2O_3, which forms dispersoids that help strengthen the alloy, also decompose to Y, which enriches the grain boundaries and contributes to cracking along the boundary. This demonstrates an important pathology in the common use of Y_2O_3 in superalloys. The panels in Figure 3 show various dispersoids along with a HAADF micrograph with the local grain boundary. In the final bottom left-hand panel, the Y-O dispersoids are in blue and the Y-Ni are in orange. Generally, the dispersoids are helpful in creep prevention, but the enhancement of the grain boundaries with Y weaken the boundary.

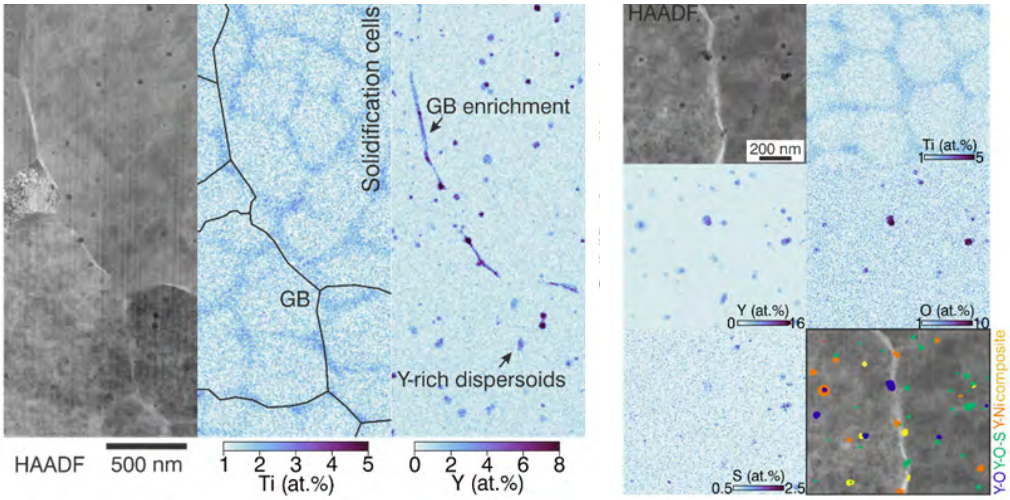


Figure 3: (Left) Grain boundary segregation of Y in the Ni-Cr-Al-Ti-Y_2O_3 microstructure. (Right) Dispersoids near grain boundary in the Ni-Cr-Al-Ti-Y_2O_3 microstructure. Courtesy of Professors Dunand and Leinenbach.

This collaborative project demonstrates the value of the ARO International Division in bringing unique international expertise to bear on U.S. Army science issues and enhancing the capabilities within the U.S. scientific community available to work on Army programs. The collaboration has been extensive and has included a number of joint papers, an NWU decision to purchase an SLM facility similar to the one at EMPA, periodic joint virtual meetings, and a long-term exchange of postdoctoral researchers.

WAY AHEAD

This project is in progress and while quantitative understanding of the processing parameter-thermal conditions-solidification behavior seems possible, there is more work to do. APT, EBSD, and TEM studies on aged and recrystallized alloys will identify the high-temperature stability and phase changes in the dispersoids alongside the formation of the precipitation strengthening phase and its interaction with the ODS dispersoids. Hot isostatic pressing will be studied as a potential post-SLM processing step to heal cracks. Hafnium(IV) oxide (HfO_2) will be studied as a potential replacement for Y_2O_3 as an oxide dispersoid.

Initial contact with ARL has expressed an interest in collaboration on SLM of an Al-based superalloy for use in unmanned aerial vehicles.

ARL Competencies:

Sciences of Extreme Materials

Results

- Demonstrated three methodologies for strengthening AM superalloys that can be employed simultaneously and in a complementary fashion.
- Showed that conventional ODS dispersoid-forming Y_2O_3 is effective but unstable under SLM conditions and deleterious to grain boundary weakening.
- Demonstrated that solidification and liquation cracking can be eliminated.
- Discovered that ductility-dip cracking along high angle grain boundaries is the dominant cracking mechanism.
- Led to extensive collaboration leveraging international expertise established for an Army basic research program.
- Led to several co-published articles between Army and university researchers, and international collaborators.

Anticipated Impact

This work is expected to provide a leap-ahead advance to the science of AM processing for DoD systems.

Computational Architecture and Visualization Program

Program Manager
Dr. J. Michael Coyle

Dr. Coyle completed his undergraduate studies at Boston College, receiving his B.A. in Mathematics in 1976. He trained as an applied mathematician at Rensselaer Polytechnic Institute, receiving his Ph.D. in Mathematics in 1990.

He came to ARO in 1999 as the Program Manager for what was then called the Discrete Mathematics and Computer Science Program.

CURRENT SCIENTIFIC OBJECTIVES

1 | Create interactive yet accurate/realistic visualizations/simulations through new theory and analysis of hybrid and acceleration techniques that combine the accuracy of numerics with the speed of computer graphics that, if successful, are anticipated to lead to enhanced training capabilities for more-effective combat readiness.

2 | Create new energy-efficient techniques and architectures for the optimal realization of multi-core systems as well as future hybrid and exascale systems that, if successful, will be able to process and operate in resource-constrained environments to support complex, resource-demanding, real-time battlefield applications.

3 | Devise scalable and communication-efficient algorithms to effectively handle the volume, heterogeneity, and multimodality of complex data arising from emerging and future Army applications that, if successful, will enable real-time, accurate delivery and analysis of critical Army data to all necessary and relevant combat units.

This success was made possible by:

Dr. J. Michael Coyle, Computing Sciences Branch

SUCCESS STORY
4D Visualization of Fire Events in Ground Vehicles

This ARO initiative resulted in the design and implementation of a customized fiber-based endoscope (FBE) setup to obtain and visualize 4D measurements of a fire event within the enclosed environment of a ground vehicle test bed. These new experimental measurements are expected to provide critical information for the improved design of future vehicles and their fire extinguishing systems for enhanced crew survivability.

CHALLENGE

While a deeper understanding of the dynamics of turbulent flames within practical applications has long been desired, it is of particular significance in the context of improving crew survivability in military ground vehicle fires. In military ground vehicles, fires can evolve rapidly and become lethal within seconds. During these situations, fire mitigation arises from vehicle design choices, and as a last resort, automatic fire extinguishing systems (AFES). Past research on fire suppression within military ground vehicles has focused on measuring, modeling, and simulating fire propagation and suppressants in order to optimize the design and application of AFES. In these studies, the focus was on the spatial and temporal development, and propagation of the flame front, an understanding of which is also of critical importance for crew survivability. To resolve these flame properties, 4D (three spatial dimensions plus time) measurement capabilities have been sorely needed to resolve the flame structure in all three spatial dimensions and also with adequate temporal resolution. However, there are key challenges toward such measurements, particularly in field applications, including hardware requirements and sufficient optical access. The equipment requirements are further compounded by the relatively hostile environments encountered in vehicular test beds.

Figure 1: Photo of the experimental setup and ground vehicle test bed, showing how the FBEs and camera were mounted on the custom frame. The locations of the nine FBEs are denoted by the numbers 1-9 in the photo. Figure courtesy of Professor Lin Ma.

ACTION

Due to a successful interaction in a previous fiscal year, Dr. Coyle was approached by an Army scientist from DEVCOM GVSC who had been working to create solutions to improving crew survivability in vehicular fires. Through discussions with DEVCOM GVSC, it became clear to Dr. Coyle that visualization capabilities of simulated fire events is a critical knowledge gap in the scientific community. After initial investigations into the field by Dr. Coyle, it was decided to leverage the expertise of Professor Lin Ma of the University of Virginia. Professor Ma is a world-renowned researcher and expert in the application of optical measurement techniques, tomography, and the experimental and analytical study of energy and thermal systems. Professor Ma was asked to create new techniques for the in situ visualization of 4D datasets and higher-dimensional datasets. It is of great interest and benefit to the Army to be able to visualize high-dimensional datasets in situ, and furthermore to guide the subsequent post-processing based on the in situ visualization. Professor Ma would then use data generated by or in tandem with DEVCOM GSVC scientists to test his theories and techniques.

RESULT

Professor Ma and his team developed a 4D imaging technique based on the combination of volumetric tomography and customized fiber-based endoscopes (FBEs). Previous volumetric tomography approaches utilized problematic methods that required multiple cameras to collect integrated line-of-sight signals, termed projections, from different orientations. The research revealed that many of these challenges can be mitigated with the implementation of FBEs in place of multiple cameras. In addition to reducing the equipment cost and simplifying the setup, FBEs have considerably smaller footprints than cameras and thus alleviate the optical access and equipment safety requirements by allowing cameras to be moved further from the volatile flame region.

A customized 9-to-1 FBE bundle was designed, where nine inputs converge to a single output, so that projections from nine different orientations can be viewed simultaneously by a single camera. The FBE was customized with an arm-length cable to reach different optical windows easily, and each input end was designed to allow lenses to be easily attached and adjusted. The new designs were field tested during a measurement campaign at ARL (Figure 1). During this campaign, the new FBE design overcame the anticipated challenges and successfully enabled 4D measurements and the associated visualization of fire events within the vehicle test bed. This is the first time that a fire event has been visualized experimentally in 4D in an Army vehicle test bed. The experimental data enabled by these measurements are expected to provide critical information to help develop and validate AFES modeling and simulation technologies for the improved design of future vehicles and their fire extinguishing systems to comply with crew safety requirements and enhance crew survivability.

WAY AHEAD

The developed methods can be extended to measure temperature and species concentration within turbulent flames, which the principal investigator will explore in future work in tandem with ARL and DEVCOM GVSC scientists, as was done in the previously described experiment. Additionally, future plans include adaptive voxel resolution to increase the speed at which the tomography process can be performed.

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

Results

- Led to co-publications between Army and academic researchers in the SAE World Congress Experience and Spring Technical Meeting of The Combustion Institute.
- Led to a joint combustion experiment conducted by ARL and academic researchers.
- Designed a new class of fiber-based endoscopes.
- Created a unique experimental setup that will greatly increase the accuracy of data for verification and validation of modeling and simulation.

Anticipated Impact

Such experimental capabilities are expected to provide new data to support the validation and development of AFES modeling and simulation in order to improve the design of ground vehicle fire extinguishing systems for enhanced crew safety and survivability, and are applicable to many different types of fires.

This success was made possible by:

Dr. J. Michael Coyle, Computing Sciences Branch

Citations:

Sathyamoorthy, A. J., Patel, U., Guan, T. & Manocha, D. *IEEE Robotics and Automation Letters*, **5**, Preprint: arXiv:2003.05395 (2020).

SUCCESS STORY

Multi-Human Multi-Robot Interactions

This ARO project developed Frozone, a novel algorithm to deal with the freezing robot problem (FRP), which arises when a robot navigates through dense environments and crowds and literally ceases to move. Such an ability allows for enhanced autonomous navigation of multiple robots on the battlefield as well as the performance of collaborative robot–Soldier tasks.

CHALLENGE

Mobile robots are increasingly used in many civilian and military scenarios, including applications such as waiters in hotels, helpers in hospitals, transporters of goods in warehouses, and reconnaissance and surveillance. To accomplish such tasks, robots need to navigate through dense and challenging dynamic environments, and crowds of people or possibly Soldiers. Apart from avoiding collisions with static and dynamic obstacles in its surroundings, the robot should also navigate in a pedestrian-friendly way. The latter includes satisfying social constraints, such as maintaining sufficient distance from the pedestrians or Soldiers, and other rules, such as avoiding them from behind. A challenging problem that a robot could face in such scenarios is FRP, which occurs when the robot faces a situation where the collision avoidance module declares that all possible paths may lead to collisions. The robot either halts or starts oscillating indefinitely, which could either result in a collision or a lack of further progress toward its goal. In practice, it is non-trivial to completely avoid FRP in densely cluttered environments or crowds of sufficient density, without human cooperation or intervention.

ACTION

In a prior fiscal year, computers scientists from the Army's Simulation, Training, and Technology Center (STTC) contacted Dr. Coyle seeking help in overcoming the challenges they faced in using modeling and simulation (M&S) techniques to train Soldiers for possible scenarios they might encounter in the future megacities combat environment. Dr. Coyle arranged and conducted a number of meetings between Professors Ming Lin (currently at the University of Maryland [UMD]) and Dinesh Manocha at the University of North Carolina at Chapel Hill (UNC) and STTC to determine the exact issues that STTC was concerned with and how Professors Lin and Manocha could be of service within the framework of an ARO basic research effort. Motivated by the practical demands of M&S, namely, a better understanding of dynamic aggregate behaviors that are observed in modern-day megacities, and being aware of their prior work on crowd modeling and robot–human interaction, Dr. Coyle saw the potential to apply such expertise to this problem. Dr. Coyle directed Professors Lin and Manocha to investigate and develop novel computational models and real-time crowd simulation algorithms that could be used for battlefield simulation, personnel training, robot interactions with crowds, and design evaluation. It was determined that many applications, such as training for battlefield simulation and urban warfare, intelligent surveillance, management of large mobs or unruly crowds, as well as the use of robots in battlefields and dangerous environments, needed improved capabilities to simulate large crowds. Such crowds are characterized based on the number of agents or pedestrians (e.g., large crowds with tens or hundreds of thousands of people), high densities, as well as heterogeneous or varying behaviors. The current state of the art is not able to model such large and diverse crowds that arise in different applications. ARO also awarded the researchers a Defense University Research Instrumentation Program (DURIP) grant at UMD to purchase robots on which to test their theories and algorithms regarding human, crowd, and robot interaction.

RESULT

Researchers at UMD developed a novel method, named Frozone, to significantly reduce the occurrence of FRP when a robot navigates through dense crowds. The approach is general and uses a standard camera for pedestrian detection and tracking. In particular, Frozone significantly reduces the occurrence of FRP by explicitly predicting pedestrian trajectories, classifying them as potentially freezing or non-freezing pedestrians, and constructing a potential freezing zone (PFZ). PFZ corresponds to a conservative spatial zone where the robot might freeze and be obtrusive to humans. They compared the performance of Frozone to three state-of-the-art techniques for robot navigation by implementing the prior methods and testing them on the robot in the same environment as Frozone. Their method successfully calculated a deviation to modify the robot's velocity to avoid the PFZ, leading to a decrease of more than 80% in freezing rates (i.e., the number of times that no freezing occurred in difficult configurations) over these prior algorithms. The method ensures that the robot's velocity avoids the PFZ and is unobtrusive to the nearby pedestrians based on their social and psychological constraints for personal space. There is a known metric for pedestrian friendliness, which is based on the study of proxemics in psychology. Ideally, the robot should maintain a safe distance from the pedestrians and not make sudden turns in front of them, which are regarded as unfriendly or uncomfortable to the humans. They used that metric to evaluate the trajectories computed using Frozone and compared them with the three state-of-the-art methods. An improvement in the pedestrian-friendliness of the robot's trajectories by 100% was observed. In addition, a state-of-the-art deep reinforcement learning-based collision avoidance method was developed and incorporated to avoid collisions with people and obstacles in dense crowds, while reducing the occurrence of freezing and guaranteeing better robustness to sensor uncertainty. The method was evaluated in simulation on a Clearpath Jackal robot and a TurtleBot (Figure 2) in several challenging indoor scenarios with crowds of varying densities. The higher fidelity of the underlying crowd simulator, also developed by this team as part of this research effort as motivated by STTC's interest in megacities, played a major role in the high performance of this learning-based robot navigation algorithm.

Figure 2: Frozone tested on a TurtleBot in dense crowds. Tests demonstrated the applicability of the method on different mobile robots with limited sensing capabilities equipped with different perception sensors. The PFZ is represented in red. Figure adapted from Sathyamoorthy et al. (2020).

WAY AHEAD

The developed method can be extended to take into account multiple robots and the dynamics constraints of the robots, which will be explored in the future potentially in tandem with STTC scientists as well as ARL CISD scientists who expressed interest during a visit to the researchers' facilities.

ARL Competencies:

Military Information Sciences

Network Science and Computational Sciences

Results

- Designed a new algorithm for FRP that leads to greatly improved robot–crowd interaction.
- Led to two publications, in *IEEE Robotics and Automation Letters* and *IEEE International Conference on Robotics and Automation*.
- Led to a visit by ARL CISD and HRED scientists to UMD lab facilities.

Anticipated Impact

Such methods are expected to provide enhanced interactions between robots and humans, and allow for the autonomous navigation of multiple robots among human crowds, as well as enhanced performance of collaborative robot–Soldier tasks, which are applicable to many different types of civilian and military scenarios including search and rescue missions.

CYBER INTELLIGENT SYSTEMS PROGRAM

Program Manager
Dr. MaryAnne Fields

Dr. Fields completed her undergraduate studies at the University of Louisville, receiving her B.S. in Mathematics in 1980. She continued her studies in Applied Mathematics at Clemson University, receiving her Ph.D. in Mathematics in 1988.

She came to ARO in 2019 as the Program Manager for what was then called the Intelligent Systems Program.

CURRENT SCIENTIFIC OBJECTIVES

1 Create new techniques in machine learning with an emphasis on online learning methods that, if successful, will provide intelligent systems the robustness, agility, and flexibility necessary to operate in complex, contested open worlds as well as the ability to create new, transferable skills to cope with dynamic and/or poorly understood situations.

2 Devise novel tools for knowledge representation, reasoning, and decision science that, if successful, will enable intelligent systems to combine knowledge from previous experiences and external sources with current observations to solve new problems and use human reasoning principles like abstraction and reflection to create new knowledge.

3 Establish principles to guide how intelligent systems interact locally with humans and other intelligent systems, remotely with spatially distant entities, and virtually in cyberspace with intelligent software agents that, if successful, will lead to new methods of human–agent and agent–agent teaming that address domains critical to the Army.

4 Develop rigorous theoretical underpinnings and practical tools for testing of unmanned systems, self-diagnosis, and risk-aware operations that, if successful, will enable assured, secure operation of intelligent systems in battlefield scenarios.

This success was made possible by:

Dr. MaryAnne Fields,
Computing Sciences Branch

Dr. J. Michael Coyle,
Computing Sciences Branch

Citations:

Hsu, J. "A Simple Neural Network Upgrade Boosts AI Performance," *IEEE Spectrum*. (2020).

Li, X., Sun, W. & Wu, T. Preprint: arXiv:1908.01259 (2019).

Wu, T. & Shipman, M. "New Data Processing Module Makes Deep Neural Networks Smarter," *NC State News*. (2020).

SUCCESS STORY
New Processing Module Improves Performance of Deep Neural Networks

Dr. Tianfu Wu, a computer scientist from North Carolina State University funded by ARO, has developed a technique to improve the performance of deep neural networks (DNNs) by combining feature normalization and feature attention modules into a hybrid attentive normalization (AN) module. This improves the classification accuracy of the system significantly while using negligible extra computational power.

CHALLENGE

In recent years, deep learning has proven to be an effective solution to many of the hard problems of artificial intelligence. But there are several challenges to applying deep learning to real-world problems encountered by future Army systems. Deep learning is becoming increasingly expensive, requiring a significant amount of computer resources to deploy object recognition and inference systems. Training (or maintaining) deep learning systems using the limited processing currently available in fielded systems is difficult. The computational cost is further increased by the way most applications are designed. Typically, new deep learning applications are built on top of existing applications that have been tuned for a particular type of problem (e.g., object recognition and natural language understanding). Reengineering such networks for better performance is challenging. Achieving the best combination of performance and resource expenditure will require researchers to rethink the underlying architecture of DNNs.

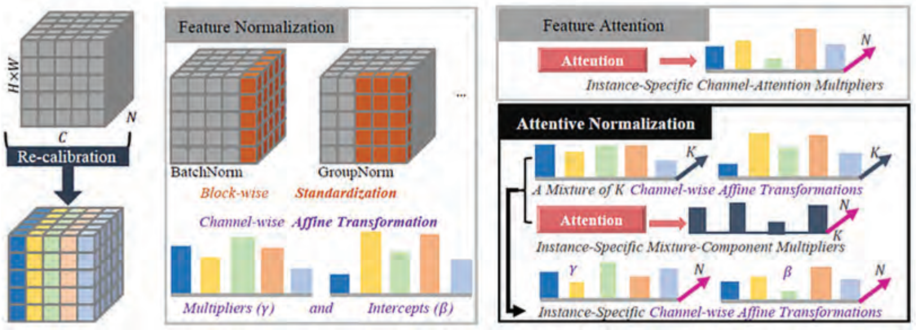


Figure 1: Illustration of the proposed AN module. AN aims to harness the best of feature normalization and feature attention. Block-wise standardization is unchanged, but AN also learns a mixture of K channel-wise affine transformations. An attention mechanism learns instance-specific weights for the mixture components, which are used in computing the weighted sum of the mixture as the final affine transformation for recalibrating the input features. Figure adapted from Li et al. (2019).

ACTION

The ARO Program Managers recruited Dr. Wu to rethink the architecture of the neural networks and develop a universal representation learning system with better parameter efficiency, interpretability, and lifelong learning capability. Since learning about his work, Dr. Fields, the Program Manager for Cyber Intelligent Systems, has assumed management of his project and worked with Dr. Wu to ensure that ARL scientists can leverage the work that he is doing. Specifically, she worked with the ARL Public Affairs Office to publicize his ground-breaking work on catastrophic forgetting, a portion of the larger project. She also facilitated meetings between ARL researchers and Dr. Wu.

RESULT

Training methods for DNNs involve two important ideas—normalization and attention. Normalization ensures that the gradients used to pass information from one layer to the next during training stay bounded so that the training process is stable and efficient. Without normalization, gradients could fluctuate wildly or become very small, making convergence difficult. Attention mechanisms improve training efficiency by providing neural networks with the ability to focus on specific subsets of the input (e.g., regions of an image). These mechanisms ensure that training procedures can account for statistical differences both between and within classes. Instead of treating normalization and attention separately, Dr. Wu took advantage of similarities between some of the computations in feature normalization and feature attention to develop an efficient hybrid module that performs both functions. Figure 1 illustrates the AN module. It preserves feature standardization, which resets the distribution for each feature in the data to have zero-mean and unit-variance, also learning a mixture of several scaling and transformation parameters. The AN module can thus be substituted for normalization components in many neural network training architectures used today. In experiments involving four representative neural architectures, including ResNet and MobileNet, Dr. Wu was able to show that the use of the AN module improved the accuracy these architectures on two industry benchmarks for object recognition and classification: ImageNet-1K and MS-COCO. Figure 2 illustrates the improvements are most significant for the MobileNet architecture, suggesting a particular advantage in computationally constrained systems.

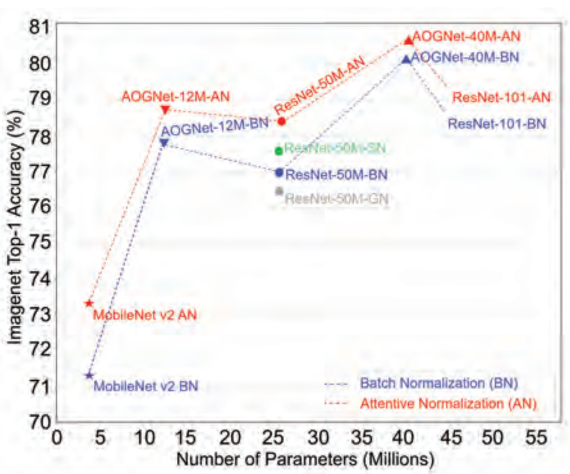


Figure 2: A comparison between the performance of five network architectures: MobileNet-v2, AOGNet-12M, AOGNet-40M, ResNet-50, and ResNet-101 using standard batch normalization and the AN module for feature normalization. Substituting AN for batch normalization consistently improves the accuracy of these architectures—MobileNet, which has the fewest parameters, shows the most significant improvement. Figure adapted from Li et al. (2019).

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

Mechanical Sciences

Results

- Presented the AN module at the 2020 European Conference on Computer Vision. Results documented in Li et al. (2019).
- Made the source code available so other researchers can experiment with the AN module and help develop better integrative designs for training DNNs.

Anticipated Impact

Both the AN module and Dr. Wu's broader efforts to redesign neural networks will lead to more efficient tools for object detection, activity recognition, natural language understanding, and other applications. These networks will improve Army systems such as robots and decision support tools. They can also enable neural networks to be used on computationally constrained systems such as embedded sensors and other surveillance devices to detect and track people, vehicles, and other objects of interest in near real time.

WAY AHEAD

The AN module is part of a broader project by Dr. Wu to rethink the architecture of the neural networks and develop a universal representation learning system with better parameter efficiency, interpretability, and lifelong learning capability. The aim is to design a family of neural architectures that can be used on many different domains or tasks in computer vision, natural language processing, or other applications of neural networks. Previous research has concentrated on developing a network structure capable of learning multiple tasks in a sequential/online manner with minimum forgetting and maximum inter-task knowledge transfer. Future technical efforts will integrate the AN module with these network structures.

This success was made possible by:

Dr. MaryAnne Fields,
Computing Sciences Branch

Dr. Purush Iyer,
Computing Sciences Branch

Citations:

Castañón, L. "Deep Neural Networks are Coming to your Phone. Here's how that could change your life," *News@Northwestern*. (2020).

SUCCESS STORY

Redesigning Deep Neural Networks for Small Processors

ARO-funded researcher Dr. Yanzhi Wang of Northeastern University developed a framework for adapting the structure of object-detection networks (e.g., You Only Look Once [YOLO]) to efficiently leverage constrained central processing unit (CPU) and graphics processing unit (GPU) resources. This enables near-real-time, state-of-the-art object detection on smartphone processors by reducing the number of calculations required.

CHALLENGE

DNNs have led to major advances in image and speech recognition, making it possible for machines to recognize faces, translate documents, and label objects in a scene. However, current systems are computationally expensive and require high-performance systems with GPU-based processors. One approach to achieve similar performance on cell phones and other small devices is to query remote high-performance computing assets. This approach is not suitable for environments with limited access to the internet, such as warzones or a disaster area. Moving DNNs to constrained processors requires compression techniques that are hardware-friendly while preserving accuracy.

ACTION

Motivated by the challenges outlined above and their implications for Army's Next Generation Combat Vehicle and Future Vertical Lift platform, Dr. Fields recruited Dr. Wang to develop techniques to compress DNNs while preserving their accuracy. Such research could remove a significant roadblock in fielding constrained autonomous systems. Dr. Fields also ensured researchers at ARL CISD were aware of this project so they could potentially use this research as they develop new artificial intelligence and machine learning algorithms for the ARL Autonomy and Intelligence for Mobility and Maneuver (AIMM) Essential Research Program (ERP).

RESULT

Many DNN models used for object detection must balance accuracy and speed. Well-known approaches, including YOLO and single shot detector (SSD), use large models that produce very accurate detections but have relatively high latency. DNNs suitable for cell phone processors sacrifice accuracy to achieve reasonable classification latency. Object-detection DNNs utilize convolutional layers that apply small mathematical filters (matrix functions) to each of the channels of an image to identify local information like edges and corners. The large number of weights that must be trained for each convolutional layer is determined by the number and size of the filters and the number of channels in the image. One promising technique for pruning. Unstructured pruning leads to the greatest compression, but often leads to inefficient computations and long inference times. Structured pruning eliminates weights in a regular manner, retaining reducing the parameter space is weight efficient computation, but often eliminates important

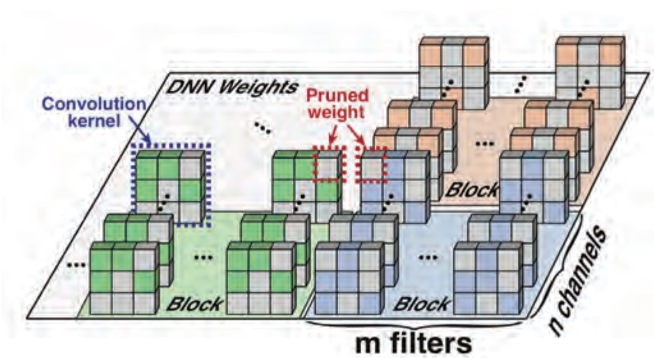


Figure 3: The block-punched pruning scheme achieves achieving high hardware parallelism while preserving classification accuracy. In this procedure, the weights from a layer of a DNN are divided into blocks with m filters and n channels by considering the characteristics of the computational resources. Weights are systematically eliminated (i.e., pruned) within a block. Figure courtesy of Dr. Yanzhi Wang.

weights, resulting in less-accurate models. Dr. Wang's team has addressed these issues by developing a novel block-pruning scheme that reduces the overall number of parameters in a network and uses a GPU-CPU collaborative scheme to improve computational efficiency on mobile devices. The block-pruning scheme, illustrated in Figure 3, divides the layer weights into equal-sized blocks of m filters and n channels, where the size of the block is chosen based on the computational characteristics of the intended hardware (e.g., length of the vector registers). Within each block, this method prunes a group of weights at the same location of all filters while also pruning the weights at the same location of all channels. Dr. Wang also developed a GPU-CPU collaborative computing scheme that improves the computational efficiency of DNNs on mobile devices.

In recent experiments, shown in Figure 4, Dr. Wang's YOLObile framework achieved a 17-fps inference speed using only the GPU on a Samsung Galaxy S20. By incorporating the GPU-CPU collaborative scheme, the inference speed is increased to 19.1 fps, five times the speed of the original YOLOv4.

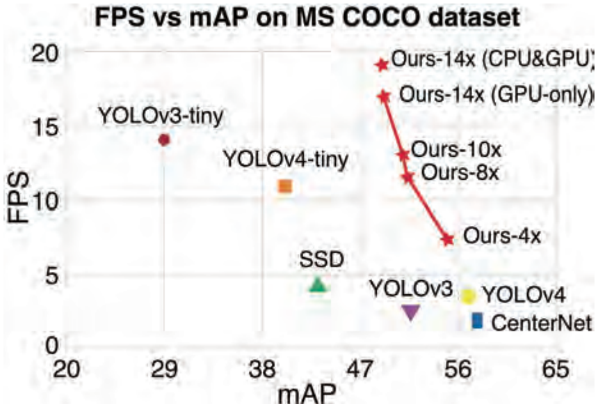


Figure 4: An accuracy (mean average precision, mAP) and speed (fps) comparison of YOLObile under different compression rates and different approaches. Figure courtesy of Dr. Yanzhi Wang.

WAY AHEAD

Dr. Wang's research has so far concentrated on the convolutional layers within a DNN. In his future work, he plans to generalize his pruning techniques to address the fully connected layers within object-recognition networks. To expand the application space, he will develop similar techniques for recurrent neural networks that have applications to speech recognition, image description generation, and text summarization. To leverage a broader range of systems, he will also extend his compression techniques to embedded processors such as field-programmable gate arrays. One potential outcome for this work is online adaptive learning on embedded processors. So far, the community has focused on inference (e.g., object recognition) from networks that have been pre-trained offline. Dr. Wang's hardware-aware implementation of DNNs may enable dynamic architectures that have the capability to adapt to new information.

Future military applications may include embedded object-recognition systems for small unmanned air and ground robots, as well as natural language processing systems suitable for Soldiers in highly restricted communication environments.

ARL Competencies:

- Humans in Complex Systems
- Network Science and Computational Sciences
- Mechanical Sciences

Results

- Led to manuscript submissions to *Journal of Solid-State Circuits* and *Proceedings on the Asia and South Pacific Design Automation Conference* (publication pending).
- Led to the team being awarded first place in the 2020 ACM/IEEE International Low Power Design Contest.

Anticipated Impact

Fast and accurate DNN inference on small/energy-constrained processors will enable future devices such as compact "smart" sensors that can be integrated into systems such as micro unmanned aerial and ground vehicles, which must operate in hostile environments with limited access to external computational resources.

INFORMATION PROCESSING AND FUSION PROGRAM

Program Manager
Dr. Hamid Krim

Dr. Krim completed his B.S. in Electrical and Computer Engineering and M.S. in Applied Mathematics at the University of Washington, and his Ph. D. at Northeastern University.

He joined ARO in 2019 as the Program Manager of the Information Processing and Fusion Program.

CURRENT SCIENTIFIC OBJECTIVES

1 | Achieve a deep understanding of data in all of its structured and unstructured forms, and discover comprehensive but simple models and algorithms that, if successful, will advance the state of the art for perception and control to enable refined decision-making for robotic agents, and help improve military and civilian security and safety through smart persistent sensing.

2 | Intelligently harvest quantitatively meaningful information from today's ubiquitous and diverse sensing of environments for a subsequent creative weaving/fusion into full scene understanding that, if successful, will enable rapid situational awareness (SA), alleviate surprise, and provide tools for a suitable response to imminent and unforeseen danger, bringing closer the reality of "anytime, anywhere" sensing autonomy for the future Army.

This success was made possible by:

Dr. Hamid Krim, Computing Sciences Branch

Citations:

Lindell, D. B. & Wetzstein, G. *Nat. Commun.* **11**, 4517 (2020).

SUCCESS STORY

Confocal Diffusion Tomography: 3D Imaging through Scattering Media

A new capability of 3D imaging through a scattering medium holds the promise of not only securing the information edge over adversaries, but also overcoming natural elements (e.g., seeing through fog).

CHALLENGE

Sensing and understanding adverse environments are central to the Army's diverse missions in the field, and exploiting the extracted information is core to successful mission completion. A significant objective of sensing-challenging environments is to maintain performance in adverse conditions, including weather (e.g., fog and rain) and other obstacles. Optical imaging carried out by light detection and ranging (LiDAR) is important in practice and essential to autonomy such as next-generation vehicles, robots, and remote sensing. Imaging an environment is hindered by the fundamental limits of the interaction of electromagnetic waves with the surrounding constituents of the environment and their resulting scattering. Such particularly difficult media include fog, rain, and dust, which have ordinarily required prior knowledge about the target location for 3D imaging to partially abate the screening effect.

ACTION

With a focused interest on multimodal sensing for understanding and inference, Dr. Krim, the ARO Information Processing and Fusion Program Manager, recognized the adverse impact of natural elements like fog and rain on sensing, and noted the existing gap in a number of sensing modalities. He encouraged Dr. Gordon Wetzstein from Stanford University to apply for the Presidential Early Career Award for Scientists and Engineers (PECASE) to provide the resources and time to pursue his research in confocal imaging in scattered media, which, in part, addressed such sensing limitations.

Intelligence distillation is the brain of the Army's mission accomplishment; sensing and gathering of associated information is the nerve that makes it work. Unimpeded sensing in an already challenging theater environment is crucial, and intelligent and possibly active sensing is increasingly necessary to mitigate natural or manmade obstruction of the scene of interest.

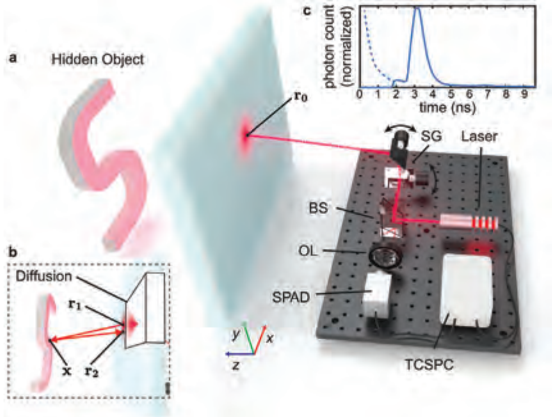


Figure 1: Schematic of 3D imaging through scattering media. Adapted from Lindell and Wetzstein (2020).

RESULT

Dr. Wetzstein, along with his graduate students, has been able to overcome challenges in multimodal sensing using single-photon avalanche diodes, ultra-fast pulsed lasers, and a new inverse method to capture 3D shapes through scattering media. This is the first such realization and was reported in a 2020 *Nature Communications* article (Lindell and Wetzstein, 2020). The technique itself couples a pulsed laser raster to a time-resolved single-photon detector. The laser scans the surface of a scattering medium shadowing the object. As light continues to diffuse through the medium, it becomes back-reflected by the hidden object and the detector captures the reflected light (Figure 1). These measurements can then be used to back-calculate the 3D shape through scattering media without a priori knowledge of the target location. Figure 2 gives an example of how the captured measurements can generate a 3D image by applying time-resolved and depth-dependent parameters to the image.

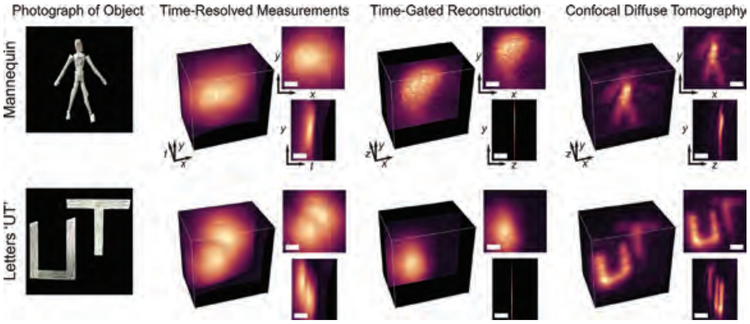


Figure 2: Overview of the 3D reconstruction through scattering media. Full details of the scattering techniques and the 3D reconstruction parameters can be found in Lindell and Wetzstein (2020).

WAY AHEAD

This research has the potential to significantly enhance sensing through obstacles (natural or otherwise), hence, augmenting autonomy capabilities including robotic applications and next-generation combat vehicles. Further research into nonstationary scattering media and other unexpected adversarial media that might arise in a battlefield will further broaden the impact on human–machine teaming and advance Army Modernization Priorities. Dr. Krim will introduce the research results to key ARL in-house researchers and establish collaborative research going forward.

SUCCESS STORY

Distributed Learning for Collaborative Fusion

This effort advanced a principled multi-domain operation with a collaboratively optimized interoperability strategy, all while maintaining a potential need for agent privacy. This could enhance SA in an adversarial environment as well as joint allied operations.

CHALLENGE

In many Army tasks, collaboration among different organizations or agents (e.g., Soldiers and other sites, mobile units) is often essential to mission success. While performing these tasks, information sharing may consist of distributed private and non-private data, situational data, and possibly a set of objectives. The distributed nature of the learner agents, together with their limited sensing capacity, and possibly additional security constraints (e.g., need-to-know) under an often adversarial environment, poses a significant challenge to harnessing the information and jointly exploiting it for an objective.

The decision of a given agent, A, often hinges on the auxiliary and appropriately integrated information of other agents to optimize performance. To provide the assistance requested by A, a remote sensing agent, B, may be querying another agent, C (e.g., a data center), which may only share, for practical reasons, a limited amount of useful information toward the initial objective of A (e.g., to determine if an approaching vehicle is a friend or foe).

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

Results

- Published a *Nature Communications* paper describing this system.
- Advanced research that could facilitate imaging in an adversarial environment and play a key role in next-generation combat vehicles.
- Demonstrated results that are a launching pad for nonstationary target imaging where the variability may be due to the scattering medium or the target.

Anticipated Impact

Dr. Wetzstein's research is expected to enable future leap-ahead technologies such as a weather-hardened next-generation vehicle and see-through-fog autonomy, with an anywhere, anytime operational capability.

This success was made possible by:

Dr. Hamid Krim, Computing Sciences Branch

Citations:

Xian, X., Wang, X., Ding, J. & Ghanadan, R. 2020 *Conference on Neural Information Processing Systems (NeurIPS), Spotlight* (2020).

ARL Competencies:

Network Science and Computational Sciences

ACTION

Distributed sensing and situational assessment, agents at geographically independent sites with diverse sensing capabilities, could provide multi-view and persistent information toward a coherent decision objective. While each agent may have a nondisclosable and private objective, the shared information remains relevant to the global objective of the mission.

This knowledge, together with the experience and interest of Dr. Krim in the area of sensor fusion and the increasingly complex environment of Army missions, led to the question of distributed intelligent fusion of information. Upon listening to one of Professor Jie Ding's (University of Minnesota) presentations on a related topic, Dr. Krim encouraged him to submit a white paper with any novel ideas in the area of collaborative information sharing. The relevance of subsequent research to artificial intelligence (AI) applications highlighted its critical importance to Army Modernization Priorities, such as autonomy and human–machine teaming, with a goal of augmenting the Warfighter's capacity to secure safety and better challenge anticipation.

RESULT

Professor Ding and his research team have developed an "active" distributed fusion methodology with the associated algorithmic and theoretical framework for actionable information. A distributed system of agents for "active fusion" in this effort is a first in its form, and with its associated practical algorithms, promises a principled and systemic acquisition of a diverse body of information broadly exploited by a distributed set of learners for distinct missions and actionable information.

This particularly useful strategy can accommodate a true collaborative solution among allied agents while each agent retains privileged information totally private. Referred to as a distributed multimodal system, its AI-based sensors can actively seek required information to accomplish a local or global objective. Any given agent, also known as a learner, is thus provided "assistance" in learning by its peers. In demonstrating the applicability of this technique to public health with a distributed set of relevant information at various locations, this technique was used to investigate the feasibility of reaching a diagnosis of a patient on the basis of such distributed information (Figure 3).

WAY AHEAD

To increase the impact on Warfighter situational information in the theater and on allied operations, in addition to developing real-time adaptive fusion with various tradeoffs and the online identification of reliable collaborating agents, the refinement of the learning foundational principles will be explored to not only enhance the privacy protection but also adapt to other Army-centric needs. Dr. Krim will also engage researchers at ARL and Army to develop and strengthen collaborative research activity with the principal investigator going forward.

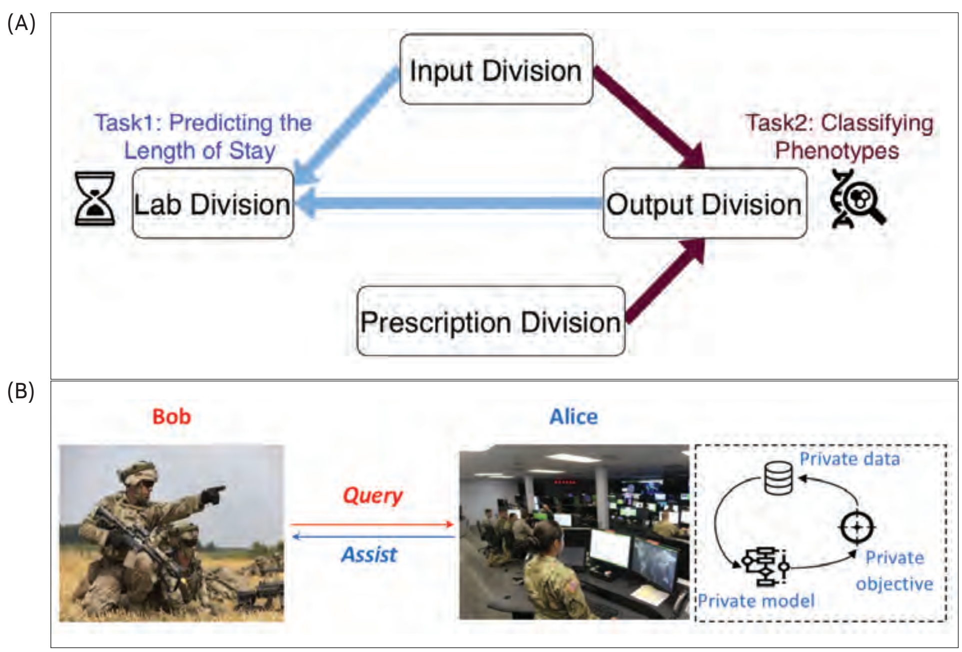


Figure 3: (A) Task-oriented active fusion among four clinical divisions, illustrated by a comprehensive clinical database MIMIC3. (B) Illustration of actionable information interchanged between a user Bob (e.g., a Soldier) and a service provider Alice (e.g., a command center), where any agent's identity may be questionable. Adapted from Xian et al. (2020).

Results

- Published a *Neural Information Processing Systems* paper in 2020.
- Shared the developed methodology and associated software with ARL CISD to potentially help manage mob-like riots in an urban setting.
- Led to the potential development of a real-time collaborative handheld tool that could be fielded to Soldiers for better tactical SA.

Anticipated Impact

Professor Ding's research is expected to enable future leap-ahead technologies such as distributed information learning and exploitation, and mission success enhancement by remote enriched information access. This could lead to more accurate SA or the ability to fuse multi-source SA from remote sensors, more quickly.

KNOWLEDGE SYSTEMS PROGRAM

Program Manager
Dr. Purush Iyer
Chief, Computing Sciences Branch

Dr. Iyer completed his undergraduate studies at the Indian Institute of Technology, Madras, receiving his B.S. in Civil Engineering in 1979. He trained as a computer scientist at the University of Utah, receiving his Ph.D. in Computer Science in 1986.

He came to ARO in 2009, after leaving his tenured professor position at North Carolina State University, and has built up programs in various aspects of artificial intelligence (AI) and network science. He is currently the Program Manager for the Knowledge Systems Program and the Institute for Creative Technologies University Affiliated Research Center (UARC).

CURRENT SCIENTIFIC OBJECTIVES

1. Develop the human-level communication that is key for the adoption of autonomous systems by large swaths of society that address issues within human communication (being structured but highly contextual) that are needed to advance natural language processing, in particular methods that employ deep learning for processing, that, if successful, will enable human–robot interaction as well make autonomous systems human-like in their interaction.

2. Advance algorithms that scale well in size yet retain their ability to look for human interaction, in the form of graphs and sub-graphs, be it the presence of adversaries in small groups within a large population or patterns of theft in financial transactions and other important questions that need to be answered to deal with both internal and external threats that, if successful, will impact social network analysis and how we deal with threats from adversarial groups in a way that is less computationally expensive.

SUCCESS STORY
Semantic Parsing using Deep Neural Networks

Until two years ago, performance of deep neural networks (DNNs) on language tasks such as parsing was considered sub-par with respect to performance on vision tasks. Over the past two years, University of Washington researcher Professor Luke Zettlemoyer, building on his prior work on semantic parsing, has constructed DNNs (the Embedded of Language Model [ELMo] and Robust Bi-Directional Language Transformers [RoBERTa]) that learn language models, from which they can create parse trees that embed contextual and relational information important for understanding language. In particular, these language models allow systems to not only understand contextual information but also generate cogent sentences. Indeed, the entire area of AI has been turned upside down by OpenAI Foundation's new Generative Pre-Trained Transformer version 3 (GPT-3), built on ideas from ELMo and RoBERTa, demonstrating a language DNN that promises to make AI systems human-like in their communication.

CHALLENGE

Statistical learning, as epitomized by DNNs, is based on correlation between inputs and outputs while ignoring the latent structure in inputs. On the other hand, natural language processing is all about uncovering the latent structure in input (e.g., sentences), which dictates the meaning of those sentences. Compositionality and phrase structure are two important principles that linguists use to explain how humans communicate and understand each other. Bringing semblance of these notions into deep learning opens up opportunities and applications for question-and-answering systems (e.g., Siri) and human–robot communication, among others.

This success was made possible by:

Dr. Purush Iyer, Computing Sciences Branch

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

Professor Luke Zettlemoyer used the opportunity afforded by the PECASE to work on the notion of bidirectional transformers, which has engulfed the natural language processing community and spurred ever-increasingly sophisticated DNNs to translate languages, such as providing answers in question–answer aides (e.g., Siri and Alexa).

ACTION

An ARO program manager can challenge the community with problems or challenge amenable individuals who are ready to address problems of importance. In this case, given that the entire community was concentrating on statistical learning, Dr. Iyer sought out Professor Zettlemoyer (University of Washington), who was working on semantic parsing that combined learning and compositional representation. Furthermore, recommending Professor Zettlemoyer for a Presidential Early Career Award for Scientists and Engineers (PECASE) in FY13, which was awarded in FY16, gave Professor Zettlemoyer the freedom to think big over a long period of time. Professor Zettlemoyer used the opportunity afforded by the PECASE to work on the notion of bidirectional transformers, which has engulfed the natural language processing community and spurred ever-increasingly sophisticated DNNs to translate languages, such as providing answers in question–answer aides (e.g., Siri and Alexa).

RESULT

Since 2017, the natural language processing community has seen a flurry of activity in a new architecture of DNNs that takes in entire sentences as input to extract order and contextual information. Importantly, what is learned from one sentence is passed back to the next layer so that contextual information is propagated. Finally, by constructing bidirectional networks, information flows not only from left to right in a sentence, but also in the other direction. The process of training such an architecture, while data hungry, has led to emergence of language models within the network, thus making it easy to construct language translators.

By collaborating with Facebook, Google, and OpenAI, Dr. Zettlemoyer's work has been imprinted in the numerous sophisticated networks that are being published every few months. Chief among Professor Zettlemoyer's contributions have been internal representations, added as an extra layer to a bidirectional network, called ELMo, which allows task-specific contextual information to be added to the network. Indeed, this representation scheme allows the same word to have two different meanings (or representations) based on the context of the sentence in which it appears. The trained model does wonderfully on the chosen tasks, thereby allowing a developer to use the bidirectional network that has been pre-trained on a large corpus. Furthermore, a group from Google published results that resulted in a system called pre-training Bi-Directional Language Transformers (BERT). BERT used ELMo as a language model, the pre-trained part, and added an additional layer that is trained on the specific application on hand.

Professor Zettlemoyer and his group, working with the Facebook AI group, showed that by training the language model (i.e., pre-trained model) on larger and vastly complicated text, the resulting BERT system would be at least an order of magnitude better; they labeled the new system RoBERTa. The developments continue in the natural language processing community, with the latest from OpenAI, in a system called GPT-3, which is capable of producing human-like text while answering questions. All of this work will lead to natural language processing systems that are capable of fully understanding human speech and writing, and translating them to other languages or answering questions.

WAY AHEAD

ARL CISD's Content Understanding Branch (CUB) is well aware of the work happening in the natural language processing community. CUB works with Professor Zettlemoyer and other researchers supported by ARO, and will transition results as they become available.

Results

- Discovered a new way of language processing that solves some of the hardest problems in natural language processing: word order and contextual semantics.

Anticipated Impact

Developing language tools to work with allied forces that speak a different language and communicating with robots in a seamless and robust fashion are some of the anticipated impacts for Soldiers.

SUCCESS STORY

Fast Identification of Triangle and k-Cliques in Large Graphs

Social media data as well telecommunications data provide a rich source of information about human activity. Identifying small adversarial groups is of significant importance for social network analysis. Professor Seshadri Comandur, University of California, Santa Cruz, has devised a series of algorithms with impressive speed ups for identifying triangles, k-cliques, and sub-graphs in graphs that are too large to be represented and explored completely (in a machine's main memory). The scientific contributions include advancement in the areas of sub-linear algorithms and probabilistic algorithms.

CHALLENGE

Social network analysis has become important, both due to the availability of data and the rise of asymmetric warfare over the past two decades. The challenge is one of searching for the proverbial needle in a haystack, for example, adversarial groups within the population of a megacity.

> **The work being done by Professor Comandur would allow the NSRL to build a suite of foundational algorithms to drive a number of analysis techniques.**

ACTION

There has been over 20 years of work in counting triangles in a graph, but without taking into account structural properties that occur in naturally occurring graphs. With the state of science in mind, Dr. Iyer recruited Professor Seshadri Comandur (University of California, Santa Cruz), a well-known theoretical computer scientist and network scientist, to work on scalable algorithms for common problems in social network analysis.

RESULT

Professor Comandur has advanced the state of science along two directions, by considering exact algorithms for a class of naturally occurring graphs and an approximate, probabilistic algorithm for all graphs. The main results were reported in a sequence of papers over the summer of 2020: (1) for graphs with low degeneracy, which include the class of random graphs that use preferential attachment (a notion propounded by Barabasi and Albert in their 1999 seminal paper), it is possible to design an algorithm that just needs to make a constant number of passes over a streaming list of edges to compute the exact number of triangles in the graph—a result that is significant as the entire graph would never have to be represented in memory, and (2) the design of a probabilistic algorithm, which works on all graphs, where it is enough to sample just a small portion of the graph (3-5%) to estimate the number of triangles fairly accurately (95% accuracy). Professor Comandur has been able to generalize these results from counting triangles to counting k-cliques, using a notion called Turán shadows–which is a tree abstraction of graph representing the recursive nature of cliques.

WAY AHEAD

Professor Comandur will be presenting a seminar at ARL CISD's Network Science Research Laboratory (NSRL) in FY21 and will be working to transition the results to the NSRL, which maintains a test bed for network science algorithms. The work being done by Professor Comandur would allow the NSRL to build a suite of foundational algorithms to drive a number of analysis techniques. Ultimately, the toolkits being constructed by the NSRL may transition to DEVCOM C5ISR.

ARL Competencies:

Network Science and Computational Sciences

Humans in Complex Systems

This success was made possible by:

Dr. Purush Iyer, Computing Sciences Branch

Results

- Discovered a new class of algorithms that would make social network analysis scalable, so that it can be applied for situational awareness in asymmetric warfare and urban warfare.

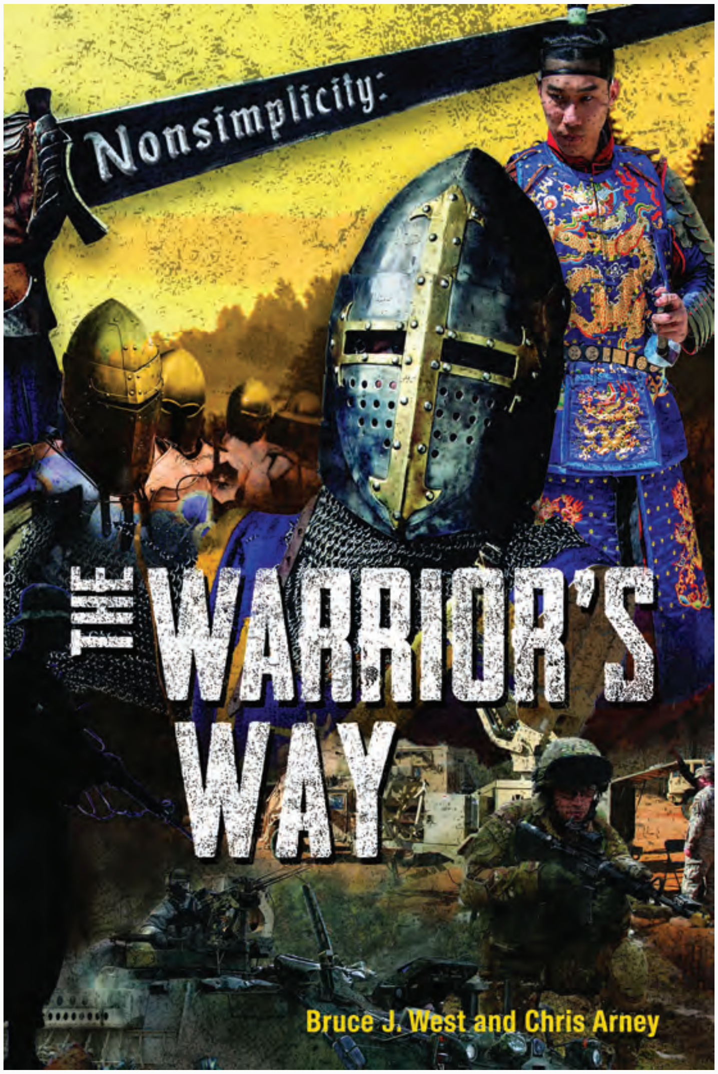
Anticipated Impact

ARL has invested over the past 10 years in network science-related algorithms and test beds to help improve situational awareness for Soldiers, fusing information from multimodal sources. The work being done by Professor Comandur would allow the NSRL to build a suite of foundational algorithms to drive a number of analysis techniques.

ARO IN THE NEWS

U.S. Army study concludes ideal network size is below 150 entities

BY GERRARD COWAN, JANE'S INTERNATIONAL DEFENCE REVIEW | SEPTEMBER 1, 2020



In the book *Nonsimplicity: The Warrior's Way*, Dr. Bruce J. West, a Senior Research Scientist at ARO, and his coauthor, retired Army Brig. Gen. Chris Arney, Ph.D., discuss how the military can grow and evolve to prepare for the future. This book is the first in a series of books being published by the *Cyber Defense Review.*

Networks of no more than 150 individuals are optimal for efficient information exchange,according to a new study by the U.S. Army Research Office (ARO), with implications in everything from training personnel to operating swarms of unmanned aerial vehicles (UAVs).

The research was conducted by ARO – an element of the U.S. Army Combat Capabilities Development Command Army Research Laboratory – in collaboration with researchers at the University of North Texas. It sought to test a hypothesis by anthropologist Robin Dunbar in the 1990s, who said that the largest group in which humans can maintain stable social relations was 150 people, with larger groups becoming unstable and breaking up into smaller groups.

The ARO-led research – published in the Proceedings of the National Academy of Sciences of the United States of America – proved Dunbar's hypothesis, showing that certain-sized networks have better information transport properties than others, with no more than 150 being the optimum size for internally sharing information as efficiently as possible.

Dunbar's work broke social groups into sizes in a "nested layering" pattern with a scaling ratio of around three – efficient groups being those comprised of 5, 15, 50, 150, and 500 people, though these are not equal in terms of the strength of relationships, according to his work. These group sizes are within a factor of two of the entity sizes of the hierarchy of the U.S. Army, noted Dr. Bruce West, senior scientist at ARO, ranging from a squad of about 15 people to a platoon of three times that size, to a company of three platoons, and so on.

The research has significant implications for armed forces, West said. For example, it could be used in training, as it suggests there are optimal sizes for learning how to function as a team member.

West pointed to retired Army Lieutenant General Stanley McChrystal in his book *Team of Teams*, which highlighted the importance of small teams having greater decision-making authority, with information being utilized where it is generated.

"If you train to utilise that information within the team, whether it's five people or 15 people, whether it's a squad or a company, you train them so that they function as a team in making decisions and using information," West told Janes . "That's the way efficient [private sector] companies operate. They don't have everything decided at the Board of Directors – where the question arises is where the answer is generated."

West said this research is applicable beyond humans, as the same findings could well be true of swarms of UAVs, in which the optimal size of a group would depend on the complexity of the swarm's mission. However, he noted that this could only be demonstrated in the future when UAVs are more autonomous.

"The 'intelligence' of any collective is size-dependent and this would also be true of swarms … the complexity of a mission would require swarms of specific size to maximise the probability of success."

Senior Research Scientist Spotlight | Dr. Bruce J. West
Senior Research Scientist, Mathematical Sciences, ARO

Dr. West graduated from the State University of New York at Buffalo with a B.A. in Physics in 1965. He graduated with a Ph.D. in Nuclear Physics from the University of Rochester in 1970, after which he was a postdoctoral researcher for two years before joining Physical Dynamics, Inc. Beginning in 1976, he served as the Associate Director and later Director at the La Jolla Institute.

Before coming to ARO, Dr. West was Professor of Physics, University of North Texas, 1989-1999; Chair of the Department of Physics, 1989-1993; and founding director of the Center for Nonlinear Science (CNS), 1994-1999. In 1992, he was elected a Fellow of the American Physical Society.

Dr. West joined ARO in 1999 as the Senior Research Scientist, Mathematical Sciences. He is a member of the American Physical Society, American Physiological Society, American Geophysical Union, American Association for the Advancement of Science, and The New York Academy of Sciences, and is an Adjunct Professor of Physics at Duke University (2000-present).

This commentary focuses on a new study by Dr. West, in collaboration with Professor Paolo Grigolini of CNS at the University of North Texas, proving a long-standing conjecture that networks of no more than 150 individuals are optimal for efficient information exchange—a principle known as the Dunbar Number in anthropology. This phenomenon has far-reaching implications for the military from operating swarms of unmanned aerial vehicles (UAVs), to training personnel to function as teams, and spans the intellectual gaps among mathematics, sociology, and psychology. In spite of the empirical evidence indicating that it does exist, there had previously been no formal theory supporting the existence of such a number.

Dr. West first came across the Dunbar Number through the popular book *Loonshots: How to Nurture the Crazy Ideas that Win Wars, Cure Diseases, and Transform Industries* by physicist Dr. Safi Bahcall (Bahcall, 2019), which was recommended to him by his ARO colleague, the Complex Dynamics and Systems Program Manager, Dr. Samuel Stanton. One of the scenarios that caught Dr. West's attention was Bahcall's discussion of the Mormon wagon trains moving west to Utah. He claimed the optimal size for a wagon train to be 150, which he justified by invoking the work of the anthropologist Professor Robin Dunbar who had reasoned that primates formed social groups that cluster at a set of magic numbers: 5, 15, 50, and 150. The number 150, Professor Dunbar hypothesized was the largest group with whom a single human can maintain a stable social relation. Near this size, the social group becomes unstable and splinters into smaller groups. What Dr. West found intriguing was the assertion that Professor Dunbar based his argument on the cognitive limitations of humans in reaching this number and that, in Professor Dunbar's opinion, this was related to the complexity of the brain.

After finishing *Loonshots*, Dr. West was interested in reading more about Professor Dunbar's theory and turned to his original text (Dunbar, 1992). In reading Professor Dunbar's papers, Dr. West began to free-associate his prose with the many conversations he had been privileged to have decades earlier with "the father of fractals," Professor Benoit Mandelbrot, who hypothesized that whenever data took the form of a scaling relation, the underlying phenomenon was fractal[1]. Though Professor Dunbar was using a different language, Dr. West surmised that he, too, was writing about scaling and that the preferred sizes of social groups he observed were the result of self-similarity. Eventually, Dr. West came across a paper in which Professor Dunbar introduced an equation, which he recognized as an allometry relation—a nonlinear scaling relation between the average functionality of a system and the average size of the system (Dunbar, 1993). Dr. West had previous research experience with allometry relations (West, 2017) and hypothesized that this was possibly the way to prove why the Dunbar Number had to be 150.

To investigate this theory, Dr. West engaged with Professor Grigolini at CNS, whose research on nonlinear science was supported by ARO's Social and Behavioral Science Program Manager, Dr. Lisa Troyer. Dr. West, Professor Grigolini, and Dr. Troyer proceeded to discuss how this empirical number was related to network science through the allometry relation and potential new applications for Professor Grigolini's research.

In Professor Dunbar's 1993 paper, the social brain allometry relation (SBAR) is the empirical source of the "magic number" 150. The equation, $N = aC^b$, relates a measure of a social quantity the average size of a primate group N, to a measure of the average size of the brain, or more accurately, a measure of the primate's cognitive function, the neocortex ratio, C. This equation provides a quantitative measure for a social property (group size) relative to an individual's psychological property (neocortical ratio), and thereby spans the gap between the individual and the collective. The empirical parameter values are $a = 1.239$ and $b = 3.389$, obtained from the best mean-square fit of a straight line to primate data. The empirical optimal size of the social group for humans is obtained by inserting the value of the neocortex ratio for humans ($C = 4.1$) into the empirical SBAR, yielding $N = 147.8$. This number was subsequently rounded to 150, what is now known as the Dunbar Number.

The fact that the number 150 is of middle range, as far as social groups are concerned, Professor Dunbar suggested is controlled by the number of minima in our neuronal landscape. How can this insight be mathematically expressed? Professor Grigolini and Dr. West wanted to develop a mathematical explanation of why $N = 150$ based on network science and the internal dynamics of interacting networks in order to understand why the number is 150 in the first place.

Dr. West and the CNS research group began with the observation that scaling occurs in the probability density function (PDF) of such a complex network and is not a property of the individual elements. Using fractional calculus, the scaling PDF is directly shown to have a first moment with the homogeneous scaling of interest necessary for establishing an allometry relation (West, 2017), and consequently, the Dunbar Number. Note that from this perspective, the scaling is a property of the group and not of the individual.

Recall that the SBAR connects a social group to a collection of neurons, thereby forming two interacting complex networks. Independently of Professor Dunbar, Dr. West and the CNS research group had some years earlier hypothesized, and subsequently proven, that the transfer of information between two interacting complex networks is dependent on the relative complexity of the two networks, and that the efficiency of the information transfer occurred when the complexity of the two networks was the same. In the decade since the resulting formalism was published (West et al., 2008), it has explained why people fall into step with one another and has been used as a rehabilitation for the age-related walking difficulties in the elderly. It has also been used to explain the distribution in the amount of time during two-person conversations that each side spoke. Each of these very different contexts has the mathematical formulation of two interacting complex networks, suggesting the use of network science to establish the value of the Dunbar Number.

The network model used in the calculation to find the Dunbar Number is based on individuals having two choices (states) and one being an imperfect imitation of the other's behavior. This decision-making model (DMM) undergoes phase transitions to reach consensus, a state of criticality in which the network changes phase. The model has emergent properties that scale and are temporally complex. In the DMM, a single individual in isolation can change opinion at a constant rate, which corresponds to having free will (West et al., 2014). To simulate a simple society, the DMM allows the agents to interact in a variety of ways and consequently the opinions of others influence the decisions of the individual. This interaction causes the transition probability to fluctuate in time, since it now depends on the states of neighbors and the strength of the coupling to them.

The DMM calculation is carried out for each value of the network size starting around $N = 50$ and sampling the network size up to $N = 5000$. The calculated PDF scales with an index α. If $\alpha = 0.5$, the process is simple diffusion, if greater than 0.5, the process is anomalous. The strength of the scaling index changes non-monotonically with increasing N and peaks at $\alpha = 0.67$ around the Dunbar Number of 150. This calculation is repeated using three distinct network models, each yielding essentially the same result (West et al., 2020). The calculation provides the first numerical evidence that the Dunbar Number is entailed by the internal dynamics of the complex networks. Further calculations indicate that 150 is the network size that has optimal information transport properties just as Professor Dunbar had hypothesized.

Subsequent calculations, not yet published, show that the same network modeling produces secondary maxima located at the network layering pattern numbers of 5, 15, 50, 150, 500, and 1,500 people. These groups are sizes within a factor of two of the entity sizes within the U.S. Army, ranging from a squad of about 15 individuals to a platoon of three times that size, to a company the size of 3 platoons, and so on. Similarly, the layering of Roman military formations from large to small was Legion (1,500), Cavalry (450 to 1,000), Century (120 to 250), Heavy Infantry (50 to 80), and Infantry (4 to 12).

The theoretical insight provided by network science supports the empirical data emphasized by Army LG Stanley McChrystal (McChrystal, 2015), who argued for teams and team-of-teams having greater decision-making authority, with information being utilized where it is collected. If one trains to utilize information within a team, the individuals function as a cognitive unit in making decisions using available information. The network science research indicates that psychological characteristics determine an individual's ability to carry out team-related tasks in the military. These psychological behavior traits may be nurtured and developed through training for the purpose of optimizing team effectiveness. In this way, the resulting teams follow the lead of efficient private companies in which answers are generated at the same place the questions arise and are not referred to a distant Board of Directors for resolution with incomplete information.

[1] *A fractal is a set of self-similar (scalable) objects (data).*

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BIOMATHEMATICS PROGRAM

Program Manager
Virginia Pasour

Dr. Pasour completed her M.S. in Biostatistics at the University of North Carolina at Chapel Hill in 1995. She trained as an Applied Mathematician at Cornell University, receiving her Ph.D. in Applied Mathematics in 2007.

She came to ARO in 2009 as the first Program Manager for the Biomathematics Program.

CURRENT SCIENTIFIC OBJECTIVES

1. Develop the mathematics and models for understanding healthy and diseased circadian rhythms that, if successful, are anticipated to lead to improved Soldier health and performance.

2. Develop the mathematics and models for understanding neurological processes related to the development and mitigation of post-traumatic stress disorder (PTSD) that, if successful, will allow the prevention and/or cure of PTSD.

SUCCESS STORY

A Quantitative Approach to the Biochronicity of Circadian Rhythm, Sleep, and Neurobehavioral Performance

This ARO initiative resulted in the development of new algorithms for optimal regulation of circadian health, which will enable improved sleep, productivity, and mitigation of the effects of traumatic brain injury (TBI).

CHALLENGE

Disruption of the circadian rhythms is known to have negative impacts on health, ranging from fatigue in travelers with jetlag, to an increased risk of cancer in rotating shift workers. Further, malalignment of the circadian phase and related neurobehavioral states, such as alertness, with the timing of critical tasks may lead to lower performance and higher risk of failure.

Regulation of circadian rhythms and the sleep process can be expressed as optimal control problems. The control inputs into the system are typically light (a strong circadian synchronizer) and chemicals such as melatonin. The objective of the optimization is to entrain the circadian rhythm as quickly as possible or maximize neurobehavioral performance during a prescribed performance interval. However, current mathematical results in the regulation of circadian rhythms do not take into account the interplay between the sleep process and the circadian process. Further, they do not include feedback from the subject. For example, optimal lighting, sleep, and pharmaceutical intake schedules are computed ahead of time and recommended to the subject prior to transmeridian travel. On the other hand, incorporating feedback into the regulation is difficult because data collection for the clinical standard markers of circadian rhythms are intrusive (through blood plasma or salivary samples), and the ensuing analysis is costly. As a result, the sampling rate is very low, at best several samples per hour, over a limited duration in experimental trials.

ACTION

While on a site visit in 2012 at Rensselaer Polytechnic Institute (RPI), Dr. Pasour heard about work Drs. John Wen and Agung Julius were doing in the area of circadian health through the Engineering Research Center on Lighting Enabled Systems and Applications (LESA) at RPI, and recognized its potential toward understanding biological clocks and contributing to the ARO Biomathematics

This success was made possible by:

Dr. Virginia Pasour, Mathematical Sciences Branch

Citations:

RPI, "A New Way to Optimize Sleep and Light Exposure Can Reduce Jet Lag and Improve Alertness," *EurekAlert!*, *AAAS*. (2019).

ARL Competencies:

Humans in Complex Systems

Biological and Biotechnology Sciences

Program's thrust in Fundamental Laws of Biology, as well as the new Defense Advanced Research Projects Agency (DARPA) program in biochronicity, for which Dr. Pasour was the contracting officer's representative. Dr. Pasour set up a meeting with Drs. Wen and Julius while on campus and discussed the fundamental biomathematical aspects in addressing the challenges in regulating circadian rhythms, sleep, and neurobehavioral processes. Convinced by the importance of addressing these mathematical challenges and their relevance to the Army, Dr. Pasour initiated a Short-Term Innovative Research (STIR) grant for Drs. Wen and Julius in December 2013. This STIR grant enabled the principal investigators (PIs) to support a part-time postdoctoral researcher and start addressing the problem for a reduced-order model of circadian rhythm dynamics.

The STIR produced several significant results, including analytical characterization of the solution to the quickest entrainment problem (i.e., how to eliminate jetlag as quickly as possible) for the reduced model and preliminary results on signal processing algorithms for biometric signals (e.g., actigraphy) in estimating the state of the subject's circadian rhythm. Based on these early results, Dr. Pasour started a new three-year Single Investigator grant in September 2017 to leverage the results of the previous work and more closely account for the interplay between sleep and circadian processes.

RESULT

The PIs were able to make significant progress on two fronts:

> **Solving optimal regulation problems for circadian rhythms and related processes:** Optimization problems involving the dynamics of circadian rhythms, sleep, and related neurobehavioral processes are complex and non-smooth, and thus hard to solve. Nevertheless, the PIs were able to develop new mathematical tools to solve problems such as determining the best lighting and sleep schedule to eliminate jetlag as quickly as possible or prepare Soldiers for a critical mission in a different time zone. An example of the computational results is shown in Figure 1.

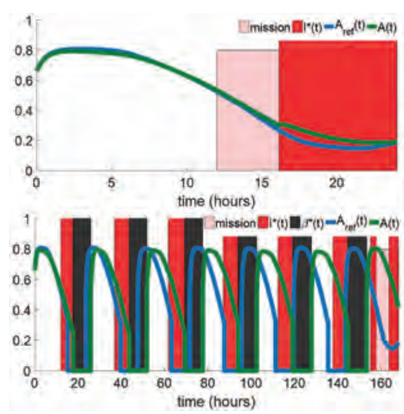
> **Using biometric signals for estimating the state of circadian rhythms and related processes:** Some of these signals are biometric data from processes that are driven by the circadian rhythms, such as actigraphy, heart rate, and body temperature. The research team demonstrated that circadian phase shift estimates obtained from processed actigraphy signals are within 1 h from those obtained using a clinical standard method.

As an unexpected side result, the PIs, in collaboration with researchers at Thomas Jefferson University, led by Dr. George Brainard, developed a method for detecting mild TBI from irregularities in the subjects' sleep quality.

WAY AHEAD

Current results are computed based on mathematical models of the circadian rhythm and neurocognitive dynamics that were derived from population average data. Thus, when used for individuals, there is certainly model mismatch. Two complementary strategies in dealing with model uncertainties in control systems are robustness and adaptation. Robustness refers to ensuring that the designed regulation algorithms work well for different models. Adaptation refers to using data to derive or tune an assumed model of the system, which is then used to design the appropriate regulation algorithms. The team plans to combine both strategies in order to harness their complementary strengths.

TBI can cause dysregulation of circadian rhythms and has been known to



Lead Time (hours)	Alertness Increase (in %)
12	5.60
36	13.7
60	29.0
84	42.2
108	53.5
132	60.0
156	62.6

Figure 1: Sample optimal solutions of the problem of optimizing lighting and sleep schedules to maximize average alertness during a 12-h mission that takes place (from 8 pm to 8 am). In the two figures on the left, the pink bands represent mission time, black bands represent optimal sleeping intervals, and red bands represent optimal lighting intervals. The green and blue curves represent the subject's optimized alertness and baseline alertness, respectively. The lead time is the amount of time between the start of the optimized schedule and the start of the mission. The top plot is for 12 h of lead time, and the bottom one is for 156 h of lead time. Both plots terminate at the end of the mission. The table on the right shows the percentage improvement of the optimized average alertness compared to the baseline (unoptimized lighting and sleep schedules). Courtesy of Drs. John Wen and Agung Julius.

Results

- Developed algorithms for optimal regulation of circadian rhythms and related processes using biometric data that can be collected using smart wearable devices.

Anticipated Impact

A quantitative approach to understanding the biological clocks inherent in circadian rhythms, sleep, and neurobehavioral performance is expected to enable data-driven personalized methods for maintaining circadian health and enhancing productivity.

"This work is important, because it characterizes the fundamental processes the human body uses to synchronize circadian and sleep processes. By developing biosensing analytics to characterize circadian phase, it is now possible to optimize the efficient use of light with appropriate spectral properties to help optimize and maintain human health and performance."

– Professor Robert Karlicek, Director, Center for LESA, Rensselaer Polytechnic Institute

impact sleep quality. Mild TBI, in particular, is also tied to chronic pain, which itself is subject to circadian rhythmicity. Thus, the study of how to regulate circadian rhythms, sleep, and the related neurobehavioral and neurological processes have the potential to help detect and mitigate the impacts of TBI. In cooperation with ARL researchers, the team plans to formulate TBI detection as a statistical decision-making problem to differentiate between two competing dynamic models (normal vs. TBI-induced dynamics). In addition, they will formulate TBI impact mitigation as an optimization problem, similar to a jetlag problem, in which the objective is to compensate for the dysregulation induced by TBI.

SUCCESS STORY

Role of Rapid Eye Movement (REM) Sleep in Emotional Memory Consolidation with Implications for Post-Traumatic Stress Disorder

This ARO initiative resulted in the development of new models for understanding and mitigating emotional memories for PTSD patients, potentially leading to evaluations of the efficacy of potential PTSD treatments.

CHALLENGE

Individuals suffering from PTSD may experience the same emotionally charged dream over and over again. Rapid eye movement (REM) sleep, the stage of sleep in which vivid dreams occur, has been implicated in the consolidation of both procedural memories (e.g., memories for the performance of motor tasks) and emotional memories. With respect to emotional memories, it is thought that REM sleep consolidates the content of the emotional memory, while at the same time reducing its emotional charge. It is known that PTSD patients have abnormal neurotransmitter levels during REM sleep. Surprisingly, we know very little about how REM sleep processes and consolidates emotional memories. The different physiological conditions under which REM sleep occurs (e.g., the levels of neurotransmitters, chemicals used by brain cells to communicate with one another), and the resulting differences in rhythmic interactions between brain areas, are thought to be critical for REM sleep-mediated emotional memory consolidation.

One standard means of deciphering the mystery of memory consolidation is to conduct animal and human experiments looking at how changes in brain connectivity during sleep relate to learning. However, considering the multiple changes that occur in the chemical environment in the intact brain during sleep, a comparison of brain connectivity changes and learning would not be easily accomplished in vitro (i.e., examining brain tissue in a dish), and the changes in brain connectivity could not be easily quantified in detail in vivo (i.e., in a behaving animal).

ACTION

The brain is one of the most mysterious yet most Army-relevant parts of the body. When Dr. Pasour arrived at ARO in 2009, toy models of the brain were finally starting to give way to more complicated realistic models. After meeting Dr. Nancy Kopell (Boston University) at a meeting at the Mathematical Biosciences Institute at Ohio State University, Dr. Pasour worked with ARO Neurophysiology of Cognition Program Manager Dr. Frederick Gregory to co-fund a proposal she submitted, including well-integrated modeling and experimental work involved in understanding complicated neural oscillations association with cognition, entitled "Prefrontal Brain Rhythms and Rule-Based Action." In 2016, Dr. Pasour attended the Society for Industrial and Applied Mathematics (SIAM) Life Sciences conference in Boston, Massachusetts, where she set up a meeting with Dr. Kopell's postdoctoral assistant, Dr. Sujith Vijayan, whose ideas on REM sleep and memory naturally built on the models and tools developed in Dr. Kopell's original grant. It became clear to Dr. Pasour that Dr. Vijayan's work had direct relevance to ARO's basic research interest in PTSD, and she encouraged Dr. Vijayan to submit a proposal for a Single Investigator grant, later awarded in 2017.

This success was made possible by:

Dr. Virginia Pasour, Mathematical Sciences Branch

Dr. Frederick Gregory, Life Sciences Branch

Citations:

Kunze, J. *SIAM News*. (2020).

ARL Competencies:

Humans in Complex Systems

Biological and Biotechnology Sciences

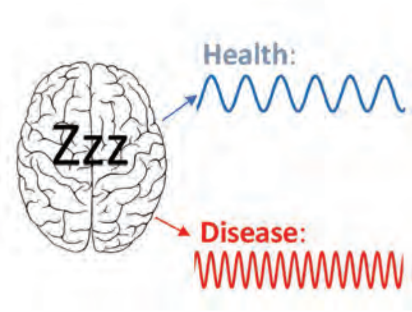


Figure 2: Insight into how aberrant neural dynamics arise during sleep may be the key to finding therapies for disorders like PTSD. REM sleep is thought to encode the content of an emotional memory while reducing its emotional charge. Rhythmic interactions (e.g., in the theta [4-8 Hz] band) between brain areas (in particular, between regions that encode emotional information and higher-order areas that encode the content of the memory) may be important for the processing of emotional memories during REM sleep. The researchers' modeling work suggests that during REM sleep, interactions between the amygdala (the main emotional center of the brain) and the prefrontal cortex could weaken the input from the amygdala to the prefrontal cortex, thus reducing a memory's emotional charge. Their work also shows that under PTSD conditions, this rhythmic activity is disrupted, thus impairing normal emotional memory processing. Courtesy of Dr. Sujith Vijayan.

RESULT

This work resulted in the development of a biophysically based mathematical model capturing both the neural dynamics observed during REM sleep and the abnormal rhythmic activity observed in PTSD patients in the key structures implicated in emotional memory consolidation. The model suggests that REM sleep reduces the emotional charge of a memory by reducing the strength of inputs from brain regions that encode emotion to the higher-order areas that represent the content of the memory (Figure 2). Using the model, the team has identified mechanisms by which the abnormal neural dynamics observed in PTSD may disrupt the normal processing of emotional memories.

WAY AHEAD

The research team will continue to refine the model as more data on PTSD neural dynamics become available. Using the model, they will probe the types of interventions that may restore normal REM sleep dynamics in PTSD patients.

In parallel with the current work, the research group has been investigating methods of altering sleep dynamics via covert auditory stimulation during sleep, which has been proven to alter sleep dynamics and enhance sleep-related learning. However, the optimal stimulus type and timing have never before been investigated. The research team has established methods for the development of an optimal stimulation paradigm. One possible "best" paradigm is currently being evaluated using sleep models (such as the one developed here) and in experimentation.

Dr. Vijayan's long-term goal is to develop acoustic sleep aids to adjust sleep architecture or enhance cognitive function in healthy individuals and restore normal sleep in patients with the disorder. The work could lead to a device that harnesses the power of sleep to better rejuvenate Soldiers or enhance their cognitive function for the completion of specific tasks. It could also be employed to prolong sleep to restore normal brain rhythms in PTSD patients or reinstate normal sleep architecture in TBI patients, alleviating the symptoms of these disorders.

Results

- Developed mathematical modeling that provided insight into the consolidation of emotional memories during REM sleep and the ways in which altered sleep physiology affects this process in PTSD patients.

Anticipated Impact

Understanding the way in which memories are processed during REM sleep will provide insight into the pathophysiology of PTSD and allow evaluation of the efficacy of potential PTSD treatments.

Computational Mathematics Program

Program Manager
Dr. Joseph Myers
Chief, Mathematical Sciences Branch

Dr. Myers has served as a logistician from platoon to brigade combat team, as a Combat Developments Officer, and on the mathematics faculty at the United States Military Academy (USMA). He holds a doctorate in Applied Mathematics from Harvard University, four Master's degrees from various academic institutions, including the Industrial College of the Armed Forces, and a Professional Engineer (PE) license.

After retirement from active duty, he joined ARO in 2008.

CURRENT SCIENTIFIC OBJECTIVES

1| Create full-scale simulations or rigorously complete simulations or summarizations in real time to investigate the behavior of systems under a variety of possible scenarios, using, potentially, reduced-order models or adaptive simplification methods based on singular value decompositions and reduced-order numerics equipped with reliable estimates of accuracy that, if successful, will enable fast and accurate modeling and simulation with an increased capability to explore the high-dimensional spaces posed by engineering design with greater fidelity.

2| Develop the mathematics for models and computational methods for anomalous physics (e.g., anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces, and finite-domain decorrelation effects) that, if successful, is expected to enable more efficient capabilities for combustion/propulsion designs, nondestructive testing capabilities for materials, and faster/more efficient engineering design.

SUCCESS STORY
Multiscale Fast and Distributed Data and Statistics Summarization

Investigations and investments in new computational geometry methods are enabling rapid information synthesis from internal high-performance computing (HPC) computations to rapid intelligence synthesis.

This success was made possible by:

Dr. Joseph Myers, Mathematical Sciences Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

CHALLENGE

The reality of modern computation is that knowledge—data—overwhelms understanding. In the course of large and complex computations or simulations, data is generally morphed, like from caterpillar to butterfly, with little opportunity to learn new connections or causal relationships of the processes at work, allowing only the opportunity to view output, do more calculations to try to determine sensitivity, and then develop heuristic models that try to reconcile our understanding with model predictions. It has been well recognized that novel methods are needed to distill or summarize large amounts of data that preserve salient features and can be utilized for subsequent analysis and visualization, both as an objective of the computation and also during the course of a computation. This problem is particularly acute when the data is both large in volume and dimension. Also, execution in scalable computing and storage environments is needed to enable parallel processing of novel algorithms that require minimal data movement. The marriage of algorithms that are widely applicable to a variety of datasets and their implementation in distributed computing environments promises to significantly reduce the time from data acquisition to knowledge discovery.

Uncovering nonlinear low-dimensional structure in high-dimensional data (i.e., manifold learning), a key to summarization, is a ubiquitous challenge across many types of applications and theory of statistics, mathematics, and machine learning. The *curse of dimensionality* is often a barrier that inhibits analysis of data in high dimensions. One consequence of working in high dimensions is that the sampling density is proportional to $N^{1/D}$, where D is the ambient dimension and N is the number of data points. Thus, a variety of analysis tasks in high dimensions (e.g., density estimation, clustering, or regression) are challenging in the ambient space. Furthermore, viable approaches to attack problems in high dimensions must scale at most linearly in the number

ARL Competencies:

Network Science and Computational Sciences

of data points and ambient dimensions to be practical for large datasets or real-time, online analysis. Algorithms must construct efficient and adaptive representations that summarize the data while preserving salient features and relationships up to a specified accuracy without amplifying noise. Finally, a barrier for many numerical methods is that their implementations are often not well suited for widespread use (i.e., their Technical Readiness Level [TRL] is low).

Broadly attacking the problem of data summarization at scale requires methods that have accuracy and scalability to guarantee applicability to a wide class of data and, from a practical point of view, requires robust implementations that can be executed on a variety of computing platforms. Of particular importance to gain widespread use are well-designed interfaces that enable integration into existing tools and support ease of use by the research community. Even "simple" numerical methods contain complex implementation issues and require significant development effort before they enjoy wide-spread adoption. Fast and well-implemented scientific computing software can enjoy wide-spread application to a variety of problems, as demonstrated by the ubiquity of the Fastest Fourier Transform in the West (FFTW) and the application of the fast multipole method (FMM) to enable significantly larger computations in molecular dynamics, celestial modeling, and scattering problems.

ACTION

ARO Computational Mathematics Program Manager Dr. Myers had started to see some successful individual efforts focused on these computational challenges, such as mathematical techniques for manifold learning and Geometric Multi-resolution Analysis (GMRA) (among others). These approaches were inspired in part by developments made in harmonic analysis but applied to data-centric problems in a novel manner. Dr. Myers saw opportunity to turn this into real capability by encouraging teaming between academia and industry, and so developed this opportunity in partnership with the ARO Technology Innovation and Outreach Branch as a Small Business Technology Transfer (STTR) Phase II topic. In the competitive offering, Intelligent Automation, Inc. (IAI) and Professor Mauro Maggioni of the University of Maryland teamed up to propose the subject effort for fast summarization, in either runtime computational data or diverse and heterogeneous collected data. Their proposal and subsequent supported project has been aimed at theoretical guarantees derived from rigorous mathematical proofs for fast runtime performance and representation accuracy, and demonstration of the benefits of the proposed approach on surrogate problems with several different types of data.

RESULT

A major accomplishment of the STTR Phase II project has been the development of a robust and scalable summarization approach. This is implemented in software and parallelized via industry-standard libraries using a technique prototyped during the Phase I effort, and leverages, with enhancements, open-source machine learning and scientific computing libraries. The software contains an automated testing suite and associated libraries can be built on many computing platforms. Benchmarks demonstrate near theoretical speed-up with the number of processing elements. GMRA-based anomaly detection algorithms have been developed, showing great promise in detecting plumes from hyperspectral movies. A robust implementation at a sufficiently high TRL enables developing summarization solutions relevant to DoD problems. Since this is mathematically based approach, it is expected to apply to a wide variety of problems. The software is expected to be sufficiently mature so that others in DoD research can utilize it, thus, increasing the impact beyond this STTR effort.

Another accomplishment made in this effort is the development of an interactive tool for visualizing and exploring summarized data. This capability is built using modern web-based elements and big data technology to support storage and access of vast amounts of data. It supports interrogation and navigation of high-dimensional data in novels ways. The visualization platform is intended to support transitions into specific problem domains, described later. Furthermore, we expect the user interface to be tailored to support transition use cases. Ongoing work has focused on application of these newly developed toolkits on additional data summarization problems and tailoring visualization capabilities to support transition use cases.

From a fundamental research point of view, this project has made significant advancements in manifold learning using the GMRA. This approach avoids the pitfalls of existing techniques, including smoothness assumptions of manifolds, poor scaling in the number of points, lack of theoretical guarantees, lack of efficient encoding of data, and lack of maps from high dimensions to low dimensions and back. The team has developed novel nonlinear techniques, inspired by diffusion

Results

- Developed a robust and scalable multiresolution approach to manifold learning.
- Demonstrated a software implementation of the manifold learning approach that is parallelized via industry-standard libraries capable of leveraging and enhancing open-source machine learning and scientific computing libraries.
- Created an automated testing suite and associated libraries that are capable of accommodating many computing platforms.
- Developed a robust implementation that is now at a sufficiently high TRL (TRL-4) to enable developing summarization solutions relevant to DoD problems.

Anticipated Impact

Multiscale fast and distributed data and statistics summarization methods are expected to enable future leap-ahead technologies such as rapid exploitation of captured documents, message resonance with target audiences, rapid design of counter strategies in response to shifts in the information space, and others.

geometry and manifold learning, for segmenting/clustering high-dimensional data in an unsupervised fashion. The data structures underlying GMRA were the key to such fast algorithms with demonstrated benefits over the current state of the art on hyperspectral images, which have millions of points in tens or hundreds of dimensions. The team has developed techniques for inference of the interaction laws in particle-agent systems, which are ubiquitous in physics, economics, and epidemiology. The team has obtained theoretically optimal estimators for pairwise interaction laws, with minimal assumptions on the form of the interaction laws, and with algorithms that scale near-linearly in the size of data. The team has developed novel algorithms for so-called "fast-slow" systems that discover low-dimensional manifolds for slow-evolving degrees of freedom in high-dimensional stochastic systems, using some of the ideas behind GMRA, and then learn effective (stochastic) equations on such low-dimensional manifolds.

WAY AHEAD

Previous research and development efforts led to novel mathematical methods and approaches that have demonstrated benefits on surrogate problems. This effort has demonstrated these approaches are viable on problem sizes of interest and sufficiently high TRL. This work has led to a transition and commercialization approach, described later, that leverages previous ARL investments and leads to deployment-relevant capabilities directly to DoD analysts. Other developments have opened the door to further fundamental research for challenging but potentially transformative advancements.

A key objective of the STTR project is the transition of advanced mathematical methods to specific problems faced by DoD and Intelligence communities. One transition path the team is preparing to pursue is Document and Media Exploitation (DOMEX) of Captured Enemy Materials (CEM) (e.g., Army Tactics, Techniques, and Procedure No. 2-91.5). When digital information is captured, analysts need tools to rapidly summarize the contents and assist in rapid exploration to discover relevant information. The GMRA-based summarization techniques hold great promise for enabling the rapid decomposition of this data for consumption and interaction by analysts, enabling analysts to more quickly discover relevant information.

Another potential capability being planned is rapid assessment of the information environment (IE), which plays an important role in the battle over "heart and minds." This is likely to help analysts quickly understand shifts in the information space and determine message resonance with the target audience. By understanding discourse shifts, analysts can better understand when counter strategies are required and can better plan for a timely deployment of these strategies. Demonstrated benefits of a multiresolution-based anomaly to detect shifts in discourse on surrogate time series have already been demonstrated. Plans are being made for incorporation into IAI's commercial product for publicly available information (PAI) analysis, Scraawl, and the deployment within Secure Unclassified Network (SUNet) enclaves. When incorporated into Scraawl/SUNet, the capabilities will become immediately available to hundreds of analysts (via a licensing model) within the U.S. Army 1st Information Operations Command, U.S. Army Intelligence & Security Command, U.S. Special Operations Command, Defense Intelligence Agency, Marine Corps Intelligence Operations Center, and other organizations. IAI will work with ECS Federal (a SUNet prime contractor) to deploy an operational prototype for end user evaluation and feedback. IAI and ECS have a history of collaboration, which will be leveraged in this technology transition.

This success was made possible by:

Dr. Joseph Myers, Mathematical Sciences Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

Citations:

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Kozak, N. *et al. Journal of Mechanics* **36**, 595-606 (2020).

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SUCCESS STORY

New Computational Methods for World-Class Engineering Modeling in Army Turbine Applications

Investigations and investments in new computational methods for engineering modeling are developing a best-in-world capability for modeling high-fidelity fluid–structure interactions as found in ARL turbine applications and elsewhere.

CHALLENGE

Geometric designs are traditionally created in computer-aided design (CAD) environments and are subsequently analyzed in computer-aided engineering (CAE) systems. Going from CAD to CAE requires a 3D mesh generation, which is labor and resource intensive, and is commonly recognized as the bottleneck in the design-through-analysis process. Furthermore, any geometric design changes guided by the computational analysis require a link from CAE back to CAD, which is nonexistent in practice. The objectives of this effort are to (1) bring together the computational fluid–structure interaction (FSI) and flow analysis from the small set of traditionally solvable problems (made feasible by bypassing certain classes of difficulties) with the classes of problems that can only be adequately modeled by including these difficult features at high fidelity, and (2) support the worldwide competitiveness of the simulation-based design, testing, and evaluation work done in the Army, DoD, and government labs by providing a capability that is unmatched anywhere in the world.

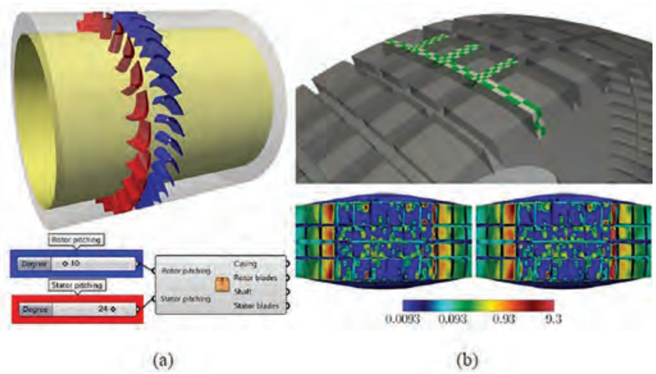


Figure 1: Multiresolution approach to manifold learning. Courtesy of YB Numerics Inc., and Professor Tayfun Tezduyar, Rice University.

ACTION

Iso-Geometric Analysis (IGA) is a new paradigm in computational sciences and engineering that aims to better integrate CAD and CAE through the use of a single geometry description for the entire design-through-analysis process. Funded by ARO and working with researchers at ARL, Dr. Yuri Bazilevs (Brown University) and his team have developed a new parametric design methodology and platform based on IGA. The platform was employed to produce parametric designs of a two-stage gas turbine model similar to that employed as part of a turboshaft for the Apache and Black Hawk helicopters and provided by ARL (Figure 1A). In addition, Dr. Bazilevs's team has developed a new method and software for high-fidelity simulation of compressible flows on moving domains. Using the parametric design framework with tight coupling to the compressible-flow software developed by the team, ARL researchers have been able to carry out parametric studies and even a formal design optimization of a two-stage turbine in support of their "articulating" blade concept. This could not have been possible without collaboration with this team and project.

RESULT

Research supported by the ARO Computational Mathematics Program has led to significant advances in, and maturing of, IGA methods for computational FSI and flow analysis, and has paved the way for a successful Army STTR Phase I project. The primary objective of this effort has been to make the meshes required for the IGA easier to generate, and thus, make the IGA more practical and more widespread in computational analysis for complex engineering applications. While this effort focuses on IGA meshing for mobility applications with significant FSI effects, the proposed IGA meshing tool, will undoubtedly make IGA more accessible for a wide range of applications. In this project, the IGA framework was deployed on the ARL single-stage gas-turbine model shown in Figure 1A. Starting with the surface geometry built using the parametric design platform and using the unique automated method described in the referenced papers, the team created a 3D IGA mesh matching the original surfaces of the gas-turbine CAD model. Results from the IGA compressible-flow computations and their comparison to the more traditional finite element simulations is shown in Figure 2. The superior boundary-layer solution quality of the IGA is clearly visible in the figure and directly translates to better predictive power of IGA.

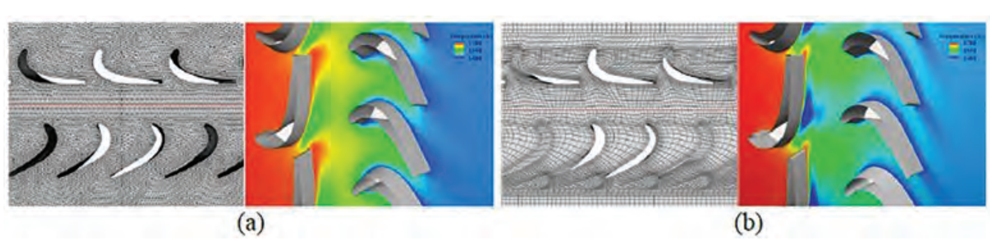


Figure 2: Cross section of a 3D mesh and temperature in the rotor-stator region of the gas-turbine stage. (a) Finite elements and (b) IGA. Sharp temperature layers smeared by traditional finite elements are accurately represented by IGA.

WAY AHEAD

In the next phase, Dr. Bazilevs and his research team aim to integrate the IGA-based design-through-analysis into a single pipeline equipped with an intuitive graphical user interface. Significant efforts are underway to partner with academia (Waseda University and Iowa State University), national research labs (Sandia National Laboratories and ARL), and industry (Simulia, Toyo Tire Corporation) to maximize the commercialization success of the proposed technology.

ARL Competencies:

Network Science and Computational Sciences

Weapons Sciences

Results

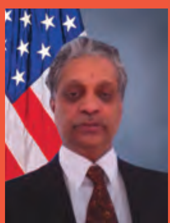
- Led to seven papers co-published between ARL and academic researchers in *Computers & Mathematics with Applications*, *Computers & Fluids*, *Journal of Mechanics*, *Energies*, and *Computational Mechanics*.
- Demonstrated that IGA consistently generates superior boundary-layer solution quality, as clearly visible in Figure 1, directly translating to better predictive power in engineering applications.
- Made significant advances in, and maturing of, IGA methods for computational FSI and flow analysis.
- Yielded a new ability to both represent the actual contact and derive high-fidelity flow solutions near the solid surfaces.

Anticipated Impact

This effort will bring new computational analysis capability for geometric complexity, actual physics, and high-quality solutions to classes of real-world problems that were never attempted before to this level of fidelity, including military and commercial mobility applications.

MODELING OF COMPLEX SYSTEMS PROGRAM

Program Manager
Dr. Radhakrishnan Balu



Dr. Balu completed his undergraduate studies at Indian Institute of Science, Bangalore, receiving his B.S. in Computer Science in 1987. He trained as a computational chemist at the University of Maryland, Baltimore County, receiving his Ph.D. in Chemistry in 2007, and joined ARL the same year. He started his research in materials science based on quantum chemistry and then branched out to quantum physics. Currently, he conducts active research in quantum computation-based artificial intelligence (AI) systems.

He was invited to join ARO in 2020 as Acting Program Manager of the Modeling of Complex Systems Program, bringing fresh perspectives from homotopy type theory and quantum information science (QIS) to the program. Dr. Balu has served in the role of technical adviser for ARO since 2017. In this capacity, he helped identify new research for the Modeling of Complex Systems Program and helped author a QIS-based Multidisciplinary University Research Initiatives (MURI) topic.

CURRENT SCIENTIFIC OBJECTIVES

1 | Develop new understanding in the geometric and topological modeling of complex systems to enable analysis, and develop an intuitive and visual picture of the underlying data that, if successful, will enable processing large-scale neuroscience data on electroencephalography and electromyography as ways of untangling brainwave activities, as well as topological analysis in combination with statistical methods that can be applied to describe phenomena from explosive events to human–machine Interactions.

2 | Develop novel modeling frameworks for analyzing streaming signals that are robust against incomplete, noisy, or dirty data that, if successful, will lead to efficient and real-time processing of brain signals in neuroscience and enable novel solutions to building new capabilities to process dynamic systems such as radars and other sensors in real time, even in the presence of noise.

SUCCESS STORY
Statistical Topological Data Analysis

This initiative on statistical topological data analysis (STDA), a broad set of techniques that are used to make inferences about the shape of data, has resulted in novel techniques to gain reliable insight about signals from complex systems by recognizing the key shape features of the signals' dynamics through oscillations over multiple resolutions and dimensions.

CHALLENGE

AI research opens up new avenues that will facilitate teams of Soldiers and AI-enabled agents to cooperate, so that tactical decisions will be made quickly and accurately. As one example, AI-enabled agents rely on analyses of Soldiers' immediate capabilities, such as immediate recall, performance of the details of intricate tasks, ability to quickly make correct identifications or appropriate judgments, ability to quickly combine facts to anticipate near-term developments, and others. These abilities are modulated by current mental and physical readiness, and the demands of the task. To that end, robust methods of analysis of the accessible physiological signals to assess a Soldier's state are required. It is anticipated that as physiological monitoring moves from the laboratory to the battlefield, physiology-based signals will become even less stationary and noisier, placing even greater challenges on current methods of analysis.

This success was made possible by:

Dr. Radhakrishnan Balu, Mathematical Sciences Branch

Dr. Joseph Myers, Mathematical Sciences Branch

Citations:

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ARL Competencies:

Humans in Complex Systems

Weapons Sciences

Citations con't:

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Townsend, J., Micucci, C. P., Hymel, J. H., Maroulas, V. & Vogiatzis, K. D. *Nat. Commun.* **11**, 1–9 (2020).

Results

- Developed R-package Bayesian topological data analysis.
- Led to students from Professor Maroulas's group collaborated with ARL HRED as summer visitors and postdoctoral fellows on this topic, helping make the work highly relevant to Army scenarios and needs.

Anticipated Impact

STDA is expected to enable future leap-ahead technologies such as automated detection of chemical compounds and efficient real-time analysis of physiological states of Soldiers.

Another challenging example is in the analysis of acoustic data when there are multiple types of explosions and varying types of resistive materials present at varying distances. In this case, automated methods for accurately identifying the explosive source type have search spaces that are both high dimensional and admit multiple parameter sets for a given observation. In both cases and others, current methodologies for analyzing these physiological and acoustic signals fall short, because they have built-in assumptions about the data they are receiving (such as stationarity, linearity, and normality). In reality, such data obeys a nonlinear rule characterized as being multimodal, multisensory, multiscale, nonlinear, nonstationary, and noisy (M^3N^3); these pose severe challenges to the development of correct and efficient solutions. New methods are required for the identification of the unique, correct parameter set that is generating the observation.

ACTION

The former Modeling of Complex Systems Program Manager, Dr. Joseph Meyer, recognized an opportunity in the works of Professor Vasileios Maroulas from the University of Tennessee. Professor Maroulas was at the forefront of incorporating topology with data analysis that enabled large datasets to be distilled into interpretable patterns. Professor Maroulas proceeded to create a classification scheme based on STDA principles, which led to a framework for developing a unique and consistent parameter set. Professor Maroulas reported this in a 2018 publication in *Advances in Data Analysis and Classification* (Marchese and Maroulas, 2018).

STDA is now showing promise in overcoming shortcomings in traditional methods to harness the information in complex physiological data efficiently that improves the Soldier's performance in the battlefield, thus surmounting the challenges in tactical decisions due to noisy data.

RESULT

Based on the success of Professor Maroulas' initial effort, Dr. Myers introduced Professor Maroulas and these STDA techniques to an ARL HRED researcher from the Context Aware Processing Branch, Dr. Tung-Duong Tran-Luu. Dr. Tran-Luu provided Professor Maroulas with a test bed of acoustic signals from two types of explosives to pose a significant test for the STDA prototype model. The problem involved automatically detecting the explosive source type, and the new method proved to be a significant improvement over existing methods. To resolve these signals in the context of cooperation between Soldiers and AI-enabled agents, the STDA solutions decreased reliance on physical constraints, but instead treated the signal as a graph or a network and then analyzed it without simplifying assumptions.

STDA is now showing promise in overcoming shortcomings in traditional methods to harness the information in complex physiological data efficiently that improves the Soldier's performance in the battlefield, thus surmounting the challenges in tactical decisions due to noisy data. The approach tackles the challenges of processing the noisy physiological data by the AI agents first by acquiring the brain signals and then applying Bayesian techniques to produce persistent diagram distributions. In the final step, the signals are successfully classified with the standard

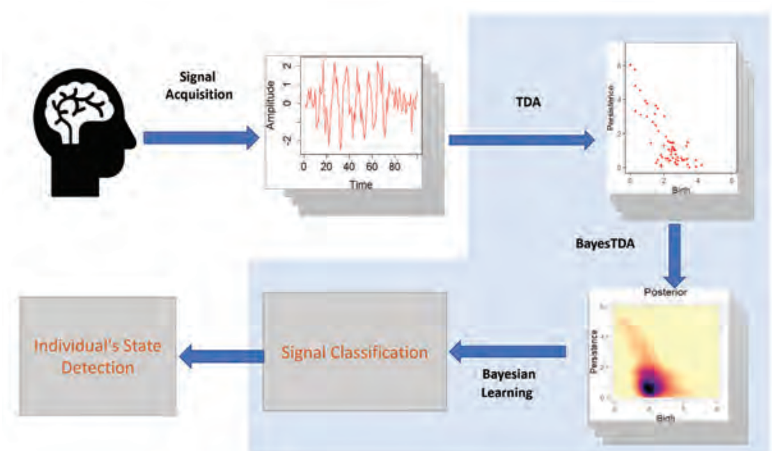

Figure 1: Statistical topological data analysis brain signals. Adapted from Nasrin et al. (2019).

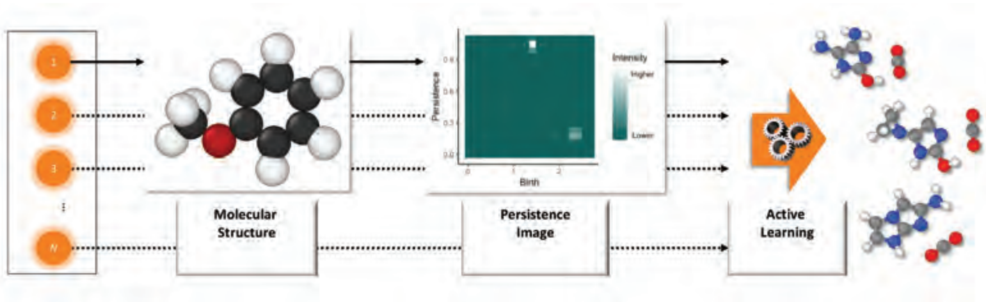

Figure 2: Molecular classification using persistent diagrams. Adapted from Townsend et al. (2020).

statistical likelihood ratio test (Figure 1). The identification of explosives proceeds by generating persistent diagrams of chemical signatures, followed by applying machine learning techniques that overcome the challenges of processing nonlinear, nonstationary, and noisy data (Figure 2). These new methods have proven much more successful in identifying the unique, correct parameter set that is generating the observation, overcoming the challenges in classifying acoustic data.

WAY AHEAD

STDA will help discover manifolds, smooth geometric objects that encode human neural states, which are hidden in certain brain activities. Such manifolds, if properly embedded within a computational neural network, could tremendously improve current machine learning algorithms as they learn to more closely emulate states of the brain. Dimension reduction leads to efficient solutions to many problems of interest to the Army and so application of STDA to such problems shows much promise.

SUCCESS STORY

Sensor Target Detection and Classification

This ARO initiative on target detection and classification is based on algebraic methods that have resulted in new avenues for the Army to pursue that can lead to modernizing the capabilities in this field. The technical developments consist of subspace tracking, preference learning, and matrix completion that form a set of abstract formalisms to base solutions for analyzing objects in a dynamical situation.

CHALLENGE

The key challenge in target detection and classification is handling massive amounts of data (e.g., streaming videos and recommender system responses) in the presence of corruption, like missing or corrupted measurements, obscured objects in a scene, or inconsistent human responses. The data streams are typically higher dimensional and identify important subspaces for realistic processing for actionable information that has heterogeneous solutions. Integrating the streams is a significant challenge. Applications of preference learning in military contexts arise whenever tasks are being prioritized, danger zones are being assessed for relative risk, and candidates are being considered for promotions or assignment to particular missions. A key machine learning advance of the last decade, and highly relevant to the problems of interest to the Army, has been the modeling of matrix-valued data with low-dimensional structures (e.g., manifolds and subspaces). There is a need to integrate such methods into dynamic data processing, and the challenge is tackled by employing abstract mathematical methods rooted in algebraic techniques.

ACTION

ARO initiated a Single Investigator grant to integrate the mathematical techniques applied in tackling the above-mentioned challenges and funded Professor Laura Balzano at the University of Michigan. She visited ARL at the beginning of this project in 2017 and consulted with several researchers, including Drs. Raju Namburu, Lance Kaplan, Alec Koppel, Ethan Stump, Brian Jalaian, and Rajneesh Singh. Briefings and discussions in this meeting further emphasized the need for novel mathematical models that can capture a wide variety of interesting phenomena seen in real data. Professor Balzano combined funding under this grant with funding from other related DoD efforts in this problem space and so formulated a comprehensive research program leveraging resources from multiple agencies.

This success was made possible by:

Dr. Radhakrishnan Balu, Mathematical Sciences Branch

Dr. Joseph Myers, Mathematical Sciences Branch

Citations:

Ongie, G., Pimentel-Alarcon, D., Nowak, R., Willett, R. & Balzano, L. *SIAM Journal of the Mathematics of Data Science* Preprint: arXiv:1804.10266 (2020).

ARL Competencies:

Network Science and Computational Sciences

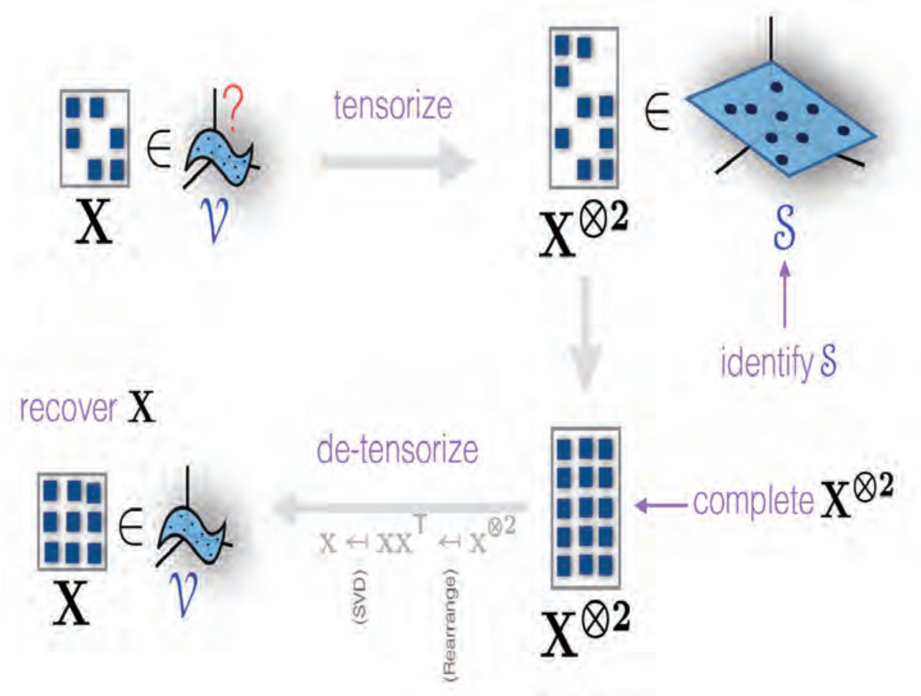

Figure 3: Integration of heterogeneous mathematical techniques to a unified framework for target detection. Adapted from Ongie et al. (2020).

RESULT

ARO investments have resulted in the development of cutting-edge techniques, such as subspace tracking, preferential learning, and data completion in information streams, all helping enable the control of dynamical systems on the fly. These advances in the "mathematics of data sciences" will potentially lead to more robust target detection in the field that is much less sensitive to anomalies in target data, clutter, incomplete or oversampled data, or other complications found in realistic use cases. To overcome the challenge of incomplete data, a larger dataset that clones the original information is generated, and by solving the corresponding algebraic equations with an assumption that they are low dimensional, the data is completed. In the last step, the missing data is identified by de-factorizing the enlarged system that recovers the "completed" original system (Figure 3). This approach has proven successful for large classes of high-dimensional streaming data.

WAY AHEAD

Next steps in this direction include creation of mathematical techniques that learn features from preference data and can identify why particular decisions are made, instead of using the existing features of the data. This will greatly improve upon current techniques, as they are often generated by deep networks or heuristic algorithms that have proven to work, but are generally uninterpretable and therefore impossible to improve in a principled way. These novel techniques can form the basis for explainable artificial intelligence (XAI) systems, whose development is significant for critical decision-making scenarios on the battlefield.

Results

- Developed techniques for unsupervised learning of a low-dimensional structure in high-dimensional messy data that is suitable for a dynamical context.

Anticipated Impact

Unsupervised, explainable machine learning techniques based on mathematical methods are expected to enable future leap-ahead technologies such as high-precision, moving-target detection and classification.

PROBABILITY AND STATISTICS PROGRAM

Program Manager
Dr. Michael Lavine

Dr. Lavine completed his undergraduate studies at Beloit College, receiving his B.S. in Mathematics in 1974. He received a M.A. in Mathematics from Dartmouth College in 1977 and a Ph.D. in Statistics from the University of Minnesota in 1987.

Dr. Lavine came to ARO in 2018 as Program Manager for Probability and Statistics after a career of more than 30 years in academia.

CURRENT SCIENTIFIC OBJECTIVES

1 | Further develop the foundations of statistical inference in the following two ways: (A) develop algorithms for finding many nearly optimal solutions to equations rather than just one, and (B) develop inferential procedures when there are several plausible models for the system being studied, that, if successful, will make the conclusions drawn from data and modelling more robust and defensible, and will help identify alternative strategies for operating convoys, swarms, communications, and fires that can adapt to local and changing conditions.

2 | Develop statistical analyses for data types that are especially relevant to the Army, such as physiological monitoring data collected in parallel from many people performing the same activity together at the same time that, if successful, will provide commanders with a more complete picture of the physiological state of their personnel to improve Soldier protection.

3 | Advance the theory of Design of Experiments (DOE) for Army-specific types of experiments to make better use of scarce experimental resources that, if successful, will enable tighter, faster design iterations of gun tubes and other computational-intensive systems.

4 | Develop approximations to, and simplifications of, the Stochastic Hybrid Systems (SHS) of equations that, if successful, will enable better understanding and control of complex and networked systems.

SUCCESS STORY
Quickest Detection

The ARO initiative produced the first mathematically accurate, non-ad-hoc results for a form of the quickest detection problem in which it is known that a change will occur in one of two channels, but it is not known ahead of time which channel will change or when the change will occur. Such problems may arise when it is believed that an adversary will choose one of several means of attack, but it is not known which one.

CHALLENGE

The problem of using ongoing observations of a stochastic process to detect as soon as possible when the probabilistic properties of the process have changed is known as the quickest detection problem. The simplest version of the quickest detection problem can be explained using the example of monitoring a single incoming channel or stream of data, even if the data is in a steady state, which is subject to random fluctuations. If the underlying state of the system changes, then the characteristics of the stream also change, which might be subject to a slow drift or an abrupt jolt, or becoming more variable. However it changes, detecting the change as quickly as possible is a high priority.

There are many variations of the quickest detection problem. For instance, monitoring many channels and wanting to detect whether there is a change in any of them or a change in a substantial number of

This success was made possible by:

Dr. Michael Lavine, Mathematical Sciences Branch

Citations:

Ernst, P. A., Peskir, G. & Zhou, Q. *Ann. Appl. Probab.* **30**, 1032-1065 (2020).

Ernst, P. A., Rogers, L. C. G. & Zhou, Q. *Stochastic Processes and their Applications* **130**, 3394-3407 (2020).

Ernst, P. A. & Rogers, L. C. G. *Mathematics of Operations Research* **45**, 1193-1620 (2020).

ARL Competencies:

Military Information Sciences

Humans in Complex Systems

Network Science and Computational Sciences

them; or monitoring a social network, where the number of nodes in the network might change over time. The way in which the data streams change might be known in advance, or might not. If we have limited monitoring capacity, we might have to choose which channels to monitor at each point in time.

Quickest detection problems with Army relevance arise in the following ways:

1. Monitoring the physiological states of a group of Warfighters over time, where each Warfighter provides a signal that undergoes normal fluctuations but that also might be subject to occasional large changes due to changes in the underlying state of the individual, while detecting changes of state as quickly as possible.

2. Monitoring air quality over time and detecting changes as quickly as possible.

3. Monitoring the health of electric batteries in a network over time and detecting abrupt changes as quickly as possible.

4. Monitoring traffic in a social network and detecting changes in both the quantity and content as quickly as possible.

In a quickest detection problem, at each point in time, a conclusion that either nothing has changed or something like channel A has changed but not channel B needs to be made. There are costs associated with failing to recognize state changes and also with falsely concluding that a channel has changed. The goal is to find a strategy for inferring changes that minimizes the total cost of both types of errors. Most strategies in the past have been ad hoc. That is, someone uses intuition and insight to propose a strategy and then verifies, with either real or simulated data, that the strategy works well and is superior to previously used strategies. The challenge for ARO is formulating good strategies based on mathematical theory rather than intuition.

ACTION

Dr. Lavine began funding research into the mathematical modeling of quickest detection problems and their optimal strategies. The development plan was to start with simplified versions of the quickest detection problem, work out the theory, and then gradually extend the theory to more complex versions of the problem. Dr. Lavine encouraged researchers to investigate and measure what is gained by putting many channels together in a single mathematical model rather than treating them individually in separate models.

RESULT

Dr. Lavine's active program management let to the publication of the first mathematically accurate, non-ad-hoc results for two variants of the quickest detection problem. In one variant, sectors of the sky were monitored because of an expected airborne attack with an unknown attack vector. Monitoring capacity is limited, so at each moment in time, a decision to determine which sector to monitor had to be made. In the steady state, the signal from each sector undergoes random fluctuations that can be well modeled by Brownian motion, but when one sector changes, its Brownian motion acquires a drift. Professor Philip Ernst of Rice University determined the optimal strategy for deciding which sector of sky to monitor and how to detect quickly when a sector becomes subject to drift. In the second variant, two data channels were monitored simultaneously. It is known that a change will occur in one of channels, but it is not known which channel will change or when the change will occur. Here, Professor Ernst determined the optimal strategy for quickly detecting when a channel has changed. The mathematical theory behind the result is based on a likelihood-ratio process. "Likelihood" is a technical term in statistics and is an underutilized way of formulating statistical problems, so the Professor Ernst's result has the additional benefit of demonstrating the value of likelihood-based inference in statistics and data science.

WAY AHEAD

The research described previously is on the mathematical formulation and solutions of quickest detection problems that have been simplified to make them mathematically tractable. The way ahead is two-fold. One way is to extend the results to more complex problems, more than two channels, different or unknown patterns of noise, or corrupted observations. Another way is to direct quickest-detection research to special problems of Army relevance. For example, if many Warfighters participate in the same activity together at the same time and, if each Warfighter

Results

- Led to several academic papers focused on problems of quickest detection published in 2020 in journals including *Stochastic Processes and their Applications*, *The Annals of Applied Probability*, and *Mathematics of Operations Research*.

Anticipated Impact

Theoretically sound use of monitors and faster detection of changes could potentially enable better situational awareness, optimal usage of battery networks, and so on.

is being monitored, we want to detect state changes in each individual Warfighter quickly and also know whether there are changes in the group's behavior that we can detect more quickly by modeling their signals collectively rather than individually.

SUCCESS STORY
Targeted Network Sampling

The ARO initiative produced an algorithm for sampling a network locally around a target node to learn which other nodes it seems to influence and a website that displays influential nodes in the Twitter network and what they are tweeting about. This has potential to quickly and automatically pick out the primary threats in target-rich environments, the leaders in large active groups, the most pressing maintenance issues in complicated systems, the key nodes in communications networks, or many others.

CHALLENGE

A new piece of information is brought to our attention in a tweet from a Twitter account. It is unknown whether the account is trustworthy, but it has to be decided quickly whether to act on the new information now or wait for confirmation. Many algorithms assess the trustworthiness of a tweet and the influence of an account by analyzing the content of the tweet and the history of the account. The challenge is to use the account's position in the Twitter network to provide additional information about its trustworthiness and influence. The position of the target account in the network encompasses such things as who the target follows, who follows the target, and even longer chains of whom follows whom.

Many methods already exist for what is called "respondent driven sampling" starting from one node in a network, then sampling from its neighbors, then from their neighbors, and so on, gradually spreading out into a random sample that represents the entire network. However, Dr. Lavine directed his focus on sampling the network heavily around the target node to learn which other nodes are closely related to the target and how strongly the target influences or is influenced by them, while also accounting for a node's popularity. There is not much information in learning that the target node follows Fox News or the New York Times because many people follow both Fox News and the New York Times. There's more information in learning that the target node follows the account of the ACLU or an obscure account in Slovenia.

ACTION

Dr. Lavine funded research in targeted network sampling and encouraged Dr. Karl Rohe, a statistician at the University of Wisconsin-Madison, to collaborate with journalists to put his sampling method into a quick and easy algorithm for users who are not expert statisticians.

RESULT

The main result of this research is the development of a new algorithm, Personal Page Rank (PPR), which makes a random walk through of a network, starting at the target. The algorithm works by sampling from the target's neighbors, then their neighbors, and so on. But whereas previous algorithms had the goal of quickly sampling as many nodes as possible and trying to move far away from the target in order to learn more about the whole network, the new algorithm incorporates a chance of returning to the target at each stage of sampling and restarting the random walk. Putting together the paths of all the random walks achieves a different purpose, namely, to sample intensively in the neighborhood of the target while simultaneously accounting for neighboring nodes' popularity (Figures 1, 2, and 3).

WAY AHEAD

Dr. Lavine is exploiting this advance within the Small Business Technology Transfer (STTR) program by developing a suitable particular scenario, possibly involving the strength of association in a given network, that could enable, as an example, using website or phone app data to enter the name of a target account and get back a list of the most strongly connected other accounts, or enter a target account and a list of other accounts and receive a measure of how closely the target is associated with accounts on the list. This targeted STTR product will be useful to journalists, investors, and other analysts who must decide whether to act on new information quickly or wait for confirmation, and will serve as one example of the far-wider range of possible applications.

This success was made possible by:

Dr. Michael Lavine, Mathematical Sciences Branch

Citations:

Chen, F., Zhang, Y. & Rohe, K. *J. R. Stat. Soc. B* **82**, 99-126 (2020).

Rohe, K. Preprint: arXiv:1505.05461 (2015).

Yan, Y., Hanlon, B., Roch, S. & Rohe, K. *Electron. J. Statist.* **14**, 1577-1610 (2020).

ARL Competencies:

- Military Information Sciences
- Humans in Complex Systems
- Network Science and Computational Sciences

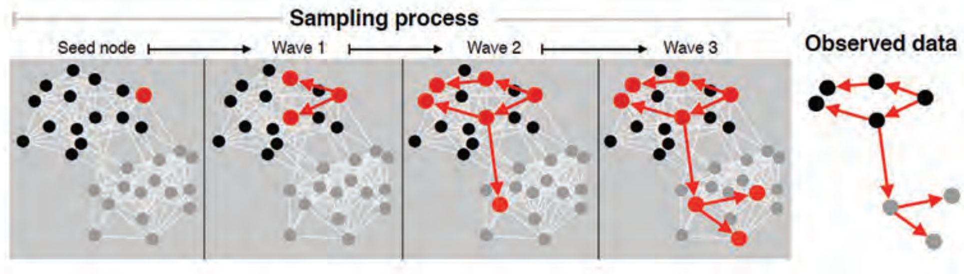

Figure 1: Traditional network sampling. Left panel: Choose a starting node (large disc). Second panel: Sample neighbors of the starting node. Third panel: Sample the neighbors' neighbors. Fourth panel: Sample the next set of neighbors and so on. Right panel: The nodes actually sampled. Adapted from Rohe et al. (2017).

Rank	*@CNN*	*@BreitbartNews*	*@dailykos*
1	CNN Breaking News	Alex Marlow	Hillary Clinton
2	CNN International	AndrewBreitbart	Stephen Colbert
3	Wolf Blitzer	Big Hollywood	Rachel Maddow MSNBC
4	Anderson Cooper	Big Government	Jake Tapper
5	Christiane Amanpour	James O'Keefe	Joy Reid
6	Pope Francis	Sean Hannity	Chris Hayes
7	Dr Sanjay Gupta	Raheem	Emma Gonzlez
8	CNNMoney	Joel B. Pollak	Markos Moulitsas
9	Jake Tapper	Ann Coulter	Maggie Haberman
10	Brian Stelter	Allum Bokhari	Sarah Silverman
11	CNN Newsroom	Ben Kew	Lin-Manuel Miranda
12	Dana Bash	Brandon Darby	Elizabeth Warren
13	CNN Politics	Noah Dulis	Jon Favreau
14	BBC Breaking News	Michelle Malkin	Michelle Obama
15	Brooke Baldwin	Nate Church	Bill Clinton

†Column names represent seed nodes, and the sampled nodes are ranked by PPR values, with teleportation constant $\alpha = 0.15$ uniformly. Through the PPR vector, the top 15 handles returned to each of the three seed nodes fit well with the characteristics of the seed nodes. They are popular or high status handles either directly related to the seed nodes or align with their political leanings. This shows the effectiveness of clustering via the PPR vector. It also shows the PPR vector's preference for highly connected nodes.

Figure 2: PPR sampling. The columns show the nodes most frequently visited by random PPR walks of the Twitter network starting from @CNN, @BreitbartNews, and @dailykos. Adapted from Chen et al. (2020).

Rank	*@CNN*	*@BreitbartNews*	*@dailykos*
1	PowerZ	Robert	Two Thanks
2	Elissa Weldon	Lee Peace	Catherine Daligga
3	Tess Eastment	Wynn Marlow	exmearden
4	Chris_Dawson	Logan Churchwell	Faith Gardner
5	carol kinstle	Peter Schweizer	Andrew Thornton
6	erinmclaughlin	Breitbart Sports	UnreasonableFridays
7	Taylor Ward	Jon Fleischman	DKos Top Comments
8	Jennifer Z. Deaton	Nate Church	2016 relitigator
9	Pam Benson	Daniel Nussbaum	Daily Kos
10	amy entelis	Noah Dulis	Walter Einenkel
11	Grace Bohnhoff	Jon David Kahn	Candelaria Vargas
12	kate lazarus	Breitbart California	Mara Schechter
13	Newstron	Ken Klukowski	Emi Feldman
14	Becky Brittain	pam key	The Soulful Negress
15	CNN Ballot Bowl	Auntie Hollywood	Kim Soffen

†Column names represent seed nodes, and the sampled nodes are ranked by adjusted PPR values, with teleportation constant $\alpha = 0.15$ uniformly. After adjustment, PPR returns a more localized cluster. Instead of the highly visible public faces of the three seed organizations, the individuals in this table serve a central role to the internal organization (e.g. editors and writers). Depending on the application, one might prefer the results in Table 1 or Table 2.

Figure 3: PPR sampling adjusted for node popularity. The columns show the nodes most frequently visited by random PPR walks of the Twitter network starting from @CNN, @BreitbartNews, and @dailykos after adjusting for each node's popularity. Compare to Figure 2. Adapted from Chen et al. (2020).

Results

- Published articles in *Journal of the Royal Statistical Society B* and *Electronic Journal of Statistics.*
- Offered a new graduate course, Modern Multivariate Statistics, at the University of Wisconsin-Madison.
- Created a new website, murmuration.wisc.edu, that displays daily the main topics of tweets from multiple groups of influential Twitter accounts.

Anticipated Impact

This advance is widely applicable, with the potential to quickly and automatically pick out the primary threats in target-rich environments, the leaders in large active groups, the most pressing maintenance issues in complicated systems, the key nodes in communications networks, and many others.

INFORMATION ASSURANCE PROGRAM

Program Manager
Dr. Cliff Wang

Chief, Network Sciences Branch

Dr. Wang received his Ph.D. in Computer Engineering at North Carolina State University.

He came to ARO in 2003 as the Program Manager for the Information Assurance Program and was promoted to Branch Chief in 2007.

CURRENT SCIENTIFIC OBJECTIVES

1. Create fundamental principles of proactive cyber defense using adaptation and deception that, if successful, could lead to new cyber-defense techniques and establish metrics for quantifying effectiveness.

2. Explore physical properties and cross-layer characteristics to derive potential new cyber-protection concepts and techniques that can complement existing methodologies that, if successful, could help build a more holistic cyber defense.

3. Establish scientific foundations for cyber autonomous systems that, if successful, may lead to establishing more-effective cyber bot–human defender teaming and defense actions in order to sustain resilient, robust, and trusted mission operations that will adopt many autonomous techniques down the road.

SUCCESS STORY

Achieving Reliability Guarantees for Critical Systems

ARO-funded research at the University of Virginia has created scalable and accurate modular analysis techniques that can detect and characterize when mission-critical system failures occur at runtime so that proactive measures can be deployed to either prevent such failures or quickly recover from their occurrences.

CHALLENGE

With the growing complexity of mission-critical systems, such as command and control or communication systems, determining and ensuring that systems will operate safely and securely when deployed is a key requirement for mission-critical applications, including Army battlefield systems. It has become ever more important to reduce the cost of safety and cyber-assurance validation while maintaining a high confidence in the validation outcome. Current approaches rely on using the best validation practices available, such as penetration testing or static vulnerability detection, and then applying human insight to carefully argue that those practices result in sufficient evidence for system reliability. While these methods can potentially expose failures, they do not provide definitive statements about system behavior. Pinpointing the failure and identifying the root cause requires extensive human intervention, making it impossible to either predict and prevent failure during runtime or recover quickly from errors when they happen. Addressing this challenge requires creating scalable and accurate modular analysis techniques that can generate explicit characterizations of system behavior to predict and detect failures, and enable on the spot recovery.

ACTION

Dr. Wang recognized the critical needs of creating runtime failure-proof systems and engaged with Professor Matthew Dwyer at the University of Virginia, who is a renowned expert in software verification, to work on the problem. Professor Dwyer has a long track record of advancing the state

This success was made possible by:

Dr. Cliff Wang, Network Sciences Branch

Citations:

Gerrard, M., Borges, M., Dwyer, M. & Fillieri, A. *IEEE Transactions on Software Engineering* (2020).

University of Virginia School of Engineering and Applied Science, “UVA professor Matthew B. Dwyer Named a Fellow by the Association for Computing Machinery,” *EurekAlert!* (2020).

ARL Competencies:

- Military Information Sciences
- Network Science and Computational Sciences

of art in software verification, such as inventing a novel technique called probabilistic symbolic execution. His work has been supported by the DoD, including an earlier Multidisciplinary University Research Initiative (MURI) on model checking for embedded systems. Through email and white paper interactions, Dr. Wang worked with Professor Dwyer to formulate the research plan and started a new project to explore automated techniques for failure avoidance at runtime.

The goal of the project was to create new software analysis techniques that can (1) predict when and where failures may happen, (2) synthesize failure avoidance logic in order to modify the state of the program to avoid potential failures, and (3) inject monitoring function to detect when failures happen at runtime and when they execute the failure avoidance logic.

RESULT

It has been challenging to incorporate the evidence provided by either dynamic or static methods into assurance arguments that are based on reliability estimates. Prior research attempting to marry abstract states with information about the probability of executing states has either been too inaccurate or too expensive. Professor Dwyer and colleagues took a completely novel approach to this problem that is inspired by conditional probability. They created conditional quantitative analysis (CQA), which combines evidence from different underlying analyses to compute bounds on failure probability. In essence, they use traditional abstract states to verify that large portions of the program's behavior are free of faults, and then they target the remaining portions with an analysis that takes into account probabilities. This allows the probability of the fault-free behavior to be computed once for each fault-free region (Figure 1); whereas, prior work requires probabilities to be computed multiple times.

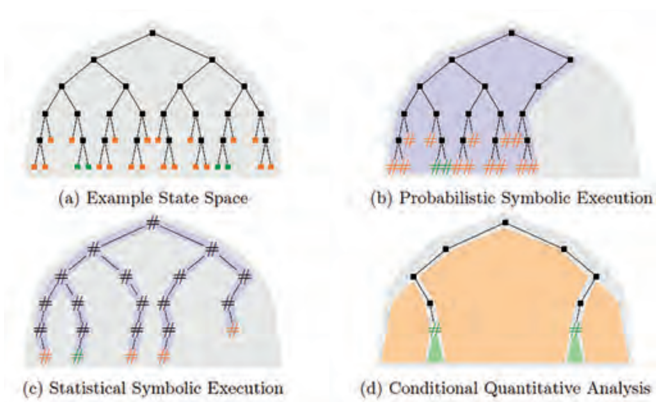

Figure 1: A comparison of CQA, developed by Professor Dwyer and colleagues, to existing state-of-the-art methods probabilistic symbolic execution and statistical symbolic execution. CQA improves on those methods by significantly reducing the number of probability calculations, depicted as "#," while guaranteeing full coverage of program behavior. Courtesy of Professor Matthew Dwyer.

The CQA technique has been developed as the alternating conditional analysis (ACA) open-source software package, which was applied to 136 C programs comprising 385k lines of source code and all with "rare faults" to test the effectiveness of the new approach. Across these programs, CQA detected hard-to-find faults at a mean occurrence probability of failure of 10-10, which is 6 orders of magnitude lower than the requirements for the most-stringent component safety integrity level defined by the international standard, International Electro-technical Commission (IEC) 61508. CQA is computationally efficient, with runtimes taking less than an hour, and can yield much higher degrees of confidence than could ever be achieved with human intervention, demonstrating the significant advancement of the state of the art.

WAY AHEAD

Professor Dwyer and colleagues continue to advance this research with support from ARO and are working to apply it to the assurance of autonomous air systems to further demonstrate its relevance and applicability. The potential Army impact of this research is the adoption of the new capability in software system behavior profiling to enable failure avoidance and error recovery to sustain mission-critical system functions. Dr. Wang will introduce A Large Portfolio-Based Alternating Conditional Analysis (ALPACA) solution that Professor Dwyer created to Army stakeholders, and help transition this advanced capability in failure detection and error recovery to enhance robustness and resiliency for many mission-critical systems such as unmanned aerial/ground vehicles, Internet of Battlefield Things, and DEVCOM C5ISR systems where real-time, uninterrupted services are expected.

Results

- Created a new software analysis tool to automate the modular application of alternating conditional analysis
- Developed the ALPACA toolset, which includes the CQA tool, now available as open-source code on bitbucket.org.
- Published the latest research outcome from the project, and the extension and application of the ALPACA toolset, in *IEEE Transactions on Software Engineering*.
- Led to Professor Dwyer being named a fellow by the Association for Computing Machinery for his pioneering work in software analysis.

Anticipated Impact

The new approach using conditional quantitative analysis will help us to build more robust and resilient mission-critical systems that can sustain its functions even when failures do occur during runtime.

SUCCESS STORY

Applying Domain Constraints for More Secure Cyber Machine Learning (ML) Systems

ARO-funded research at Pennsylvania State University has created new machine learning (ML) analysis algorithms that led to the first adversarial sample generator capable of incorporating domain constraints, which can be used to carry out effective assurance tests of cyber ML systems.

CHALLENGE

ML is an emergent technology that has been transforming our society. However, like any other cyber system, ML applications are shown to be vulnerable from adversarial exploits. Malicious inputs could be designed to drive unexpected worst-case behavior when a ML system is not adequately protected. Although recent adversarial ML (AML) research has studied the security issue, most research focuses on the image/video domain. For the cyber domain, ML systems such as network intrusion detection, threats, and defense mechanisms are drastically different from image or language domain applications. One of the hard problems is to understand the effects and influence of key factors such as domain constraints and dimensionality that are unique for the cyber domain, and critical for building robust and resilient cyber systems.

ACTION

Dr. Wang identified the critical issue of ensuring the security of ML systems. The emergent research area is quite often called AML. In 2017, Dr. Wang teamed up with Professor Patrick McDaniel (Pennsylvania State University) to organize a special workshop on AML research, one of the earliest, at Stanford University to identify research challenges. In 2019, Dr. Wang and Professor McDaniel served together as co-chairs to lead a national Artificial Intelligence and Cybersecurity workshop organized by the National Science and Technology Council's (NSTC) Networking and Information Technology Research and Development (NITRD) Subcommittee. The resulting workshop report identified key research challenges at the intersection of AI and cybersecurity, and generated critical research investment strategy recommendations. In the same time frame, Dr. Wang supported Professor McDaniel to study key issues, such as transferability, dimensionality, and domains, critical to AI system robustness and resiliency, and establish the metrics that can help define and ensure trustworthy ML-based systems in practice.

RESULT

Adversarial input through carefully planned data manipulation has shown to be able to severely disrupt deep learning-based systems, such as video processing systems for autonomous driving. While many research efforts have tackled this problem in the image/video domain, little research has been done in the cyber domain, where attack models and feature assumptions are quite different. Cyber features can often be measured from varying sources, representing complex relationships and interdependencies. Also in the cyber domain, unlike performing image perturbation with few limitations, there are many features that an adversary has no control over, such as timing-based features (e.g., round-trip times) or host-based features (e.g., the rate at which a destination host is sending information). It is unclear how these domain idiosyncrasies affect vulnerabilities in black-box threat models. To tackle this problem, Professor McDaniel and his collaborators first studied the feature space of cyber ML systems to understand domain constraints and their influence on the input space. By leveraging algorithms from the formal logic community to identify, extract, and incorporate domain constraints into the adversarial data sample crafting process, they created an innovated approach as follows: (1) formalizing domain constraints as a set membership problem, (2) generating a universe of possible relationships as an allowable set, (3) extracting domain constraints using modified Valiant's algorithm, and (4) incorporating the obtained minimum set into crafting adversarial examples. Using the Davis–Putnam–Logemann–Loveland (DPLL) algorithm, which is a complete, backtracking-based search algorithm for deciding the satisfiability of propositional logic formula in conjunctive normal form, Professor McDaniel built the first algorithm to craft adversarial examples in constrained domains.

Dubbed as constrained saliency projection (CSP), the algorithm can be used to generate perturbed inputs to cause misclassification. This new approach was applied to six real-world datasets, spanning areas including network intrusion detection, malware detection, phishing, and medicine, for analysis of attack space and ML system resiliency (Figure 2). The results show that domain

This success was made possible by:

Dr. Cliff Wang, Network Sciences Branch

ARL Competencies:

Military Information Sciences

Network Science and Computational Sciences

Results

- Participated in the Artificial Intelligence and Cybersecurity: A Detailed Technical Workshop, NITRD.
- Created the first algorithm, called the CSP tool, to generate adversarial examples in constrained domains.
- Shared and transitioned results to ARL CISD with a joint publication being prepared.
- Led to Professor McDaniel being elected to Fellow of the American Association for the Advancement of Science (AAAS), cited for distinguished contributions to the field of computational security and privacy.

Anticipated Impact

The novel method of generating cyber domain-specific adversarial examples will enable defenders to perform more comprehensive penetration test to ensure the safety, security, and trustworthiness of cyber ML systems, especially DoD systems enabled by ML technologies.

constraints can sometimes substantially limit the available space exploitable by adversaries, thereby presenting a vastly different threat model than previously understood. By being able to create a unique threat model catered to the specifics of the domain under investigation, the new method fixed a major flaw of previous work where specifics of a domain are commonly not captured. Also, the ability to generate domain-constrained samples allows defenders to perform comprehensive penetration test effectively to ensure ML systems are well prepared for malicious exploits.

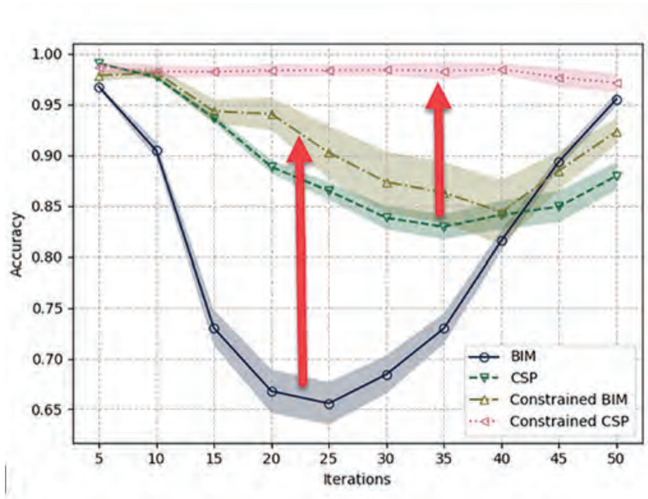

Figure 2: The model accuracy pre- and post-projection in constrained domains. The team benchmarked their approach against the state of the art in unconstrained domains, the basic iterative method. The results show that domain constraints can "pull back" adversarial examples outside of the attack space (indicated by the arrows), greatly enhancing the classification accuracy of ML systems. Courtesy of Professor Patrick McDaniel.

WAY AHEAD

Professor McDaniel will continue his work to explore adversarial examples in other security-centric domains to ensure ML system security. The team will build a space of threat models to allow security practitioners to verify first and then deploy ML systems in ways that they can be trusted in the presence of an adversary. The potential Army impact of this research is that the curated threat models returned by crafting adversarial examples in constrained domains will help cyber defenders to identify all potential attacks more precisely and help reduce response time to enhance mitigation. ARL scientists are actively collaborating on the project to further mature the technology for transition to the Army.

MULTI-AGENT NETWORK CONTROL PROGRAM

Program Manager
Dr. Derya Cansever

Dr. Cansever completed his undergraduate studies at Bosphorus University, receiving his B.S. in Electrical Engineering in 1979. He trained as an electrical and computer engineer at the University of Illinois at Urbana-Champaign, receiving his Ph.D. in Electrical and Computer Engineering in 1985.

He came to ARO in 2017 as the acting Program Manager for the Communications and Hybrid Networks Program and is currently the Program Manager for the Multi-Agent Network Control Program.

CURRENT SCIENTIFIC OBJECTIVES

1 | Determine the fundamental limits of, and develop methods for, distributed control in large networked systems that, if successful, will support efficient and effective implementations of the Army's goal of distributed mission control, without losing sight of the common goal that drives its operations.

2 | Develop methods for learning in networked control systems, such as multi-agent reinforcement learning that, if successful, will drastically enhance the operational capabilities of Army's autonomous systems and protect our Soldiers from high-risk environments.

3 | Develop control methods that ensure the stability of quantum systems, such as reliable qubits, that, if successful, will enable quantum computations that can have transformative effects such as breaking previously unbreakable codes and solving optimizations problems of unprecedented scales.

SUCCESS STORY

Verifiable Reinforcement Learning in Networked Systems

This ARO initiative has shown that it is possible to develop theory and algorithms for verifiably safe and policy-compliant reinforcement learning in networked autonomous systems that operate in dynamic, uncertain, and possibly adversarial environments.

CHALLENGE

Reinforcement learning is a research area that is fundamental to the operation of autonomous systems, a crucial component of future Army systems. Using operationally obtained and simulated data, reinforcement learning can direct the operation of autonomous systems. However, because of the unpredictability of human supervision, system complexity, and possible data contamination, safety and policy compliance of reinforcement learning systems cannot always be guaranteed. Without proper and effective mitigations, this could lead to potential vulnerabilities in the game-changing capabilities that reinforcement learning can provide.

ACTION

Dr. Cansever identified reinforcement learning, and in particular, its safety and policy compliance as an important research areas for the Army. He met with Professor Ufuk Topcu, an expert in decision learning at the University of Texas at Austin, at a decision and control conference. They had a discussion on open research problems in reinforcement learning. After hearing Professor Topcu's vision and ideas on this topic, Dr. Cansever encouraged him to submit a white paper to ARO on the safety of reinforcement learning. The white paper and the ensuing proposal eventually led to an ongoing ARO project: "Verifiable Reinforcement Learning in Networked Systems."

This success was made possible by:

Dr. Derya Cansever, Network Sciences Branch

Results

- Successfully tested the shield system, establishing reinforcement learning benchmarks with no noticeable performance impairment.
- Demonstrated the proposed algorithms to be effective in realistic scenarios that involved 50 agents over a simulated battlespace environments.

ARL Competencies:

Network Science and Computational Sciences

Anticipated Impact

The resulting algorithms are expected to contribute to the Army's mission by shortening the time needed for the deployment of autonomous systems in the field, increasing their mission effectiveness, and elevating the level of resources the adversaries need to expend to counter the Army's capabilities.

This success was made possible by:

Dr. Derya Cansever, Network Sciences Branch

Citations:

Xu, J., Sun, Y., Tian, Y. & Scutari, G. Preprint: arXiv:1910.09817 (2019).

RESULT

This project addresses the gap in our ability in developing adaptable yet provably correct autonomous systems through a merger between reinforcement learning and formal methods. Formal methods offer clear semantics for reasoning about correctness. Learning-based algorithms introduce adaptation to contextual changes and incompleteness of information at time of design. To address the need to incorporate formal methods in the decision system, and implement safety and policy in the resulting actions, Professor Topcu developed a shield system that is responsible for monitoring the decisions by the learning algorithm with respect to satisfying safety and mission-critical specifications, and correcting these decisions only when necessary (Figure 1).

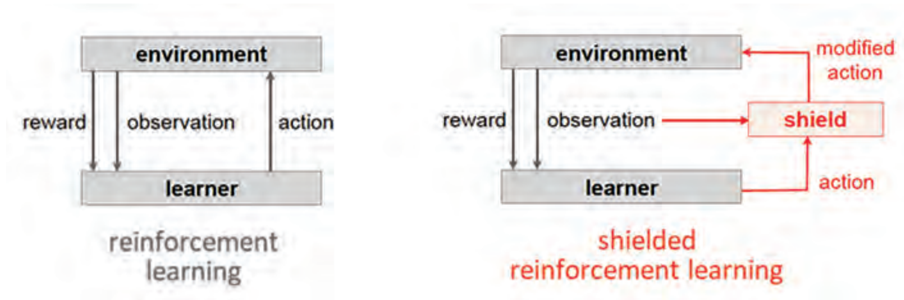

Figure 1: Illustration of shielded reinforcement learning. Courtesy of Professor Ufuk Topcu.

Simulations and laboratory experiments indicated that shielded reinforcement learning provides provability, guarantees safety, and scales independently of the inner workings of the learning algorithm. The proposed solution works with a large variety of learning algorithms, facilitates system integration and compositionality, and offers robustness to contextual variations. The algorithm was tested on multiple multi-agent reinforcement learning benchmarks and improved scalability was observed without affecting the performance.

WAY AHEAD

Professor Topcu and his research team are creating a pipeline (in synergy with other U.S. Army Futures Command-funded efforts) to demonstrate the resulting algorithms on ARL's autonomy software stack and Phoenix simulator.

SUCCESS STORY

Distributed Robust Nonconvex Optimization over Time-Varying Networks: Tradeoffs and Guarantees

This ARO initiative has resulted in a new, unified convergence and performance analysis of distributed algorithms based on novel operator splitting techniques. This effort has identified the methods that distributed control techniques use to match the performance of centralized control in heterogeneous swarm networks. The proposed approach has been adopted by the community as a standard procedure to study the behavior of prominent distributed algorithms.

CHALLENGE

Networks of swarms are becoming increasingly important for the Army. In making swarms operationally feasible, an enormous challenge is how to design distributed algorithms for control, optimization, and learning with no centralized agents and large numbers of heterogeneous assets. One of the goals is to match or come close to the performance of centralized operation when assets do not have access locally to the totality of the relevant information. One needs to identify the best achievable tradeoffs in solution accuracy, computation, and communication overhead. Also, critical considerations include how to make the algorithms robust against network variability, attacks, and asynchronous modus operandi.

ACTION

ARO scientists recognized the value of distributed control of swarm network systems for the Army and invested in several projects in this area. Professor Gesualdo Scutari from Purdue University was one of the initial researchers encouraged to submit a proposal in this area, which led to a successful project on distributed robust nonconvex optimization over time-varying networks. Dr. Cansever met with Professor Scutari in 2020 to discuss the types of swarm networks relevant to the Army and the underlying mechanisms used in their control. This research topic has the potential to further inspire novel control mechanisms in networked systems.

RESULT

Professor Scutari and his research group designed a distributed optimization algorithm achieving fast convergence and accurate solutions over time-varying networks, such as a network of agents that acts as a swarm (Figure 2). These algorithms do not require any centralized information-gathering agent. The algorithms they designed matched the performance of centralized optimization algorithms. Professor Scutari and his research group demonstrated fast convergence of their algorithms, and also showed that the algorithms are effective in environments where data is exchanged asynchronously and airwaves are contested. The proposed novel in-network optimization and signal tracking mechanism makes up for missing information by delivering accurate estimates in many cases of interest. Their approach proved to be not only sufficient to achieve the desired optimal performance, but also necessary to be included in any other decentralized algorithm to be effective. As a result, their approach has become a standard procedure as an agreed-upon benchmark in the evaluation of the distributed control algorithms.

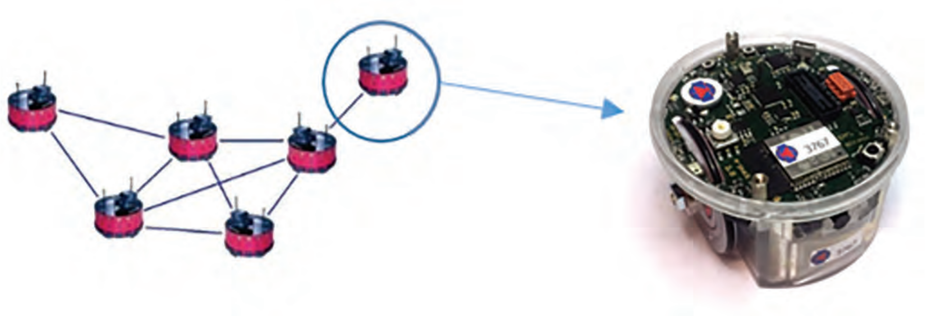

Figure 2: Laboratory demonstration of the controlled swarm network. Courtesy of Professor Gesualdo Scutari.

Secondly, Professor Scutari and his research group have shown that to design provably fast, reliable, and robust algorithms, one needs to go beyond currently used consensus-based schemes and enable more sophisticated in-network tracking mechanisms to estimate locally missing global information. They have shown an important result that a speedup of algorithmic convergence can be achieved with respect to centralized optimization if communications are properly balanced with local optimization steps. They also established that communications protocols should not be designed independently from the optimization algorithms, as was done in the prior state of the art.

WAY AHEAD

Future research will lead to a new statistically informed optimization theory and algorithmic design, revealing new fundamental limits, guarantees, and tradeoffs, resulting in globally optimal, distributed algorithms. If successful, this is expected to transition to ARL to support and complement ongoing research in swarm networks.

ARL Competencies:

Network Science and Computational Sciences

Results

- Won the Best Paper Award at the 2019 IEEE International Workshop on Computational Advances in Multi-Sensor Adaptive Processing for "A Unified Contraction Analysis of a Class of Distributed Algorithms for Composite Optimization."
- Developed fast converging and accurate distributed algorithms for time-varying, random swarm networks that can match the performance of centralized optimization algorithms.

Anticipated Impact

The resulting algorithms are expected to simplify and make more efficient the control and operation of swarms of networked elements that support Army operations.

SOCIAL AND COGNITIVE NETWORKS PROGRAM

Program Manager
Dr. Edward T. Palazzolo

Chief (Acting), Physics Branch

Dr. Palazzolo completed his undergraduate studies in 1997 at the State University of New York at Buffalo as a double major in Psychology and Communication. He received his M.A. from the State University of New York at Buffalo in Interpersonal and Organizational Communication in 1999. He earned his Ph.D. at the University of Illinois Urbana-Champaign in 2003 in Organizational Communication and Knowledge Management.

He came to ARO in 2014 as the Program Manager for the Social and Cognitive Networks Program.

CURRENT SCIENTIFIC OBJECTIVES

1| Discover the fundamental principles governing human teaming activities that support designing and maintaining high-performance teams that, if successful, will allow the Army and Joint Staff to engineer high-performance teams with specified characteristics to satisfy mission requirements and enable teaming with unprecedented coordination across multiple defense organizations, while improving Soldiers' cognitive resilience.

2| Create verifiable models of networked human behavior by bridging social science theories with computer science techniques and engineering precision that, if successful, will create the ability to forecast societal opinions and shifts with pinpoint accuracy, especially with potential for real-world effects, to support Army and Joint Operations by providing support for decision-making.

3| Create new social network research methods and analytics to handle the challenges associated with novel and advanced research in team science and computational social science that, if successful, will enable deeper understanding of the complex human terrain in Multi-Domain Operations.

This success was made possible by:

Dr. Edward T. Palazzolo,
Network Sciences Branch

SUCCESS STORY
Building Cognitive Resilience in Human–Agent Teams

This ARO initiative developed strong competencies for cognitive resilience in human–agent teams (HATs). Dr. Leanne Hirshfield at the University of Colorado Boulder's Institute of Cognitive Science created a custom test bed with integrated reinforcement learning system for HAT data collection through the observation of the team states of human participants performing information analysis tasks with an embedded artificial intelligence (AI) team member.

CHALLENGE

There are two primary scientific challenges necessary to overcome for creating an ecologically valid test bed for studying HATs. First, the research team must design and develop the physical environment, including sufficient instrumentation and biosensors for the study of human behavior and cognition. Second, they must collect sufficient training data for reinforcement learning to build a suitable agent robust enough for human interaction within the test-bed environment.

For this line of research, Dr. Palazzolo specifically uses the word "agent" to indicate that teaming is between humans and computer systems (an AI) with agency (as opposed to computers as tools, such as remote operated or autonomous vehicles). From this perspective, agents have the ability to make decisions and control situations in a similar way in which humans can. Moreover, agents can be responsible for task assignments and prioritizations of human activities. Therefore, it is imperative that we build theoretical models based on valid testing environments to understand the ways in which humans will not only respond to such agents, but how HATs can be substantially more effective than human-only teams.

ACTION

Dr. Palazzolo built part of his portfolio around research that supports the Army's need for cognitive resilience. As explained in U.S. Army Field Manual (FM) 7-22 "...resilient Soldiers can better leverage mental and emotional skills and behaviors that promote enhanced performance and optimize their long-term health." Dr. Palazzolo built on the strong findings of the "Mind-Body-Community Connections" research program highlighted in the 2019 ARO Year in Review, which focused on the cognitive impact of the social networks with which people surround themselves and mitigation strategies, such as mindfulness and hypnotherapy, on peer influence. Adding to that line of research, he supported a research program led by Dr. Hirshfield and Dr. Sidney D'Mello at the University of Colorado Boulder's Institute of Cognitive Science. Along with other efforts, these programs established a strong concentration of research on HAT in support of the Army's future warfighting needs for Multi-Domain Operations (MDO) and beyond.

During the white paper phase, Dr. Palazzolo discussed the above perspective for studying HATs with Dr. Hirshfield while she was still a professor at Syracuse's Newhouse School of Public Communication. She was identified as the best researcher to pursue this line of work based on her focus on the use of noninvasive cognitive and physiological measurement to passively classify user states for usability testing and adaptive system design. Her extensive research portfolio focuses on the use of physiological sensors for predicting users' social-cognitive-affective states for use in the field of human–computer interaction. This new grant advances that line of research into team science. Further, Dr. Palazzolo added to their conversation his preference for a study of trust in teams that is consistent with Stephen M. R. Covey's framework for Speed of Trust, which focuses on the credibility (made up of character and competence) of the individual and high-trust behaviors between individuals, such as creating transparency. Dr. Hirshfield incorporated these concepts into the design of her research test bed and has laid the ground work for studying swift trust within these teams.

RESULT

Dr. Hirshfield developed a theoretical framework to suggest appropriate human states of interest, system adaptations, and evaluation criteria, focused on calibration of trust and reliance in HATs. She created a prototype intelligent trust modulation (ITM) system, using a reinforcement learning system architecture, to calibrate human teammate trust and reliance during collaborative HAT tasks.

To test her theoretical framework with the ITM system, she successfully created a custom HAT test bed with an integrated reinforcement learning system for human subjects data collection. The test bed has the capability to observe both individual and team states, has an embedded AI for agent interactions, and its interface can be augmented to (1) conduct task shedding when human team members are in a hazardous mental state, (2) change AI transparency for proper trust and reliance, and (3) change information overlays about team member credibility in order to build swift trust. The testing screen for human interaction with accompanying agent interactions is shown in Figure 1. To observe and assess individual states, participants are outfitted with a suite of high-fidelity biosensors (Figure 2) including galvanic skin response, eye tracking, and functional near-infrared spectroscopy (fNIRS). Additionally, the test bed allows for unobtrusive observations using more traditional computer science methods such as sensors for facial recognition, voice, and speech patterns for discourse analysis. Collectively, these sensors, when fused over all participants on the team, allow for an assessment of the team state and changes in team states over the course of the teaming activities, such as in this research scenario working together to place crime prevention resources around Denver, Colorado. The custom test bed and data collections are designed to formulate and train a reinforcement learning system (via a partially observable Markov decision process) to sense relevant team states and execute appropriate actions to calibrate team trust and reliance.

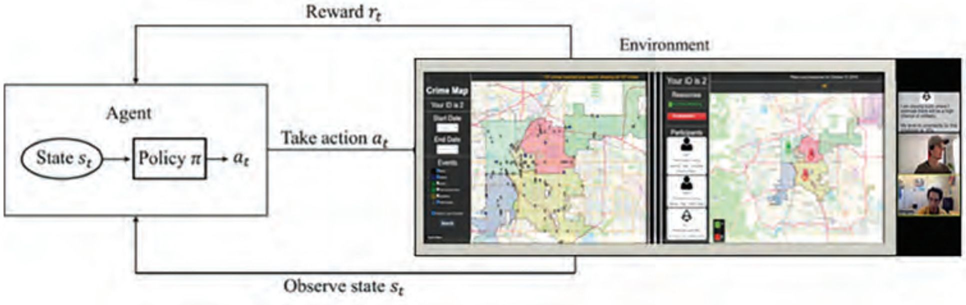

Figure 1: Example of the research training environment with source data on the left screen, an individual human teammate and agent teammate data on the right. Courtesy of Drs. Leanne Hirshfield and Sidney D'Mello.

ARL Competencies:

- Military Information Sciences
- Humans in Complex Systems
- Network Science and Computational Sciences

Results

- Developed an experimental test bed for the study of HATs with an emphasis on swift trust and cognitive resilience.
- Enabled Tri-Service coordination and contributions to basic research on HATs.

Anticipated Impact

If successful, this research will lead to enhanced capabilities for Army intelligence analysts working in teaming environments with respect to (1) enabling AI coordination and tasking with humans and (2) maintaining analytic integrity through periods of cognitive decline and cognitive overload. Additionally, this work has potential for enhancing cognitive resilience in teaming environments such as Mission Commands and Joint Staffs.

Figure 2: Example of a research participant with biosensors (including fNIRS, galvanic skin response, and heart-rate monitor) in a split screen view of individual and HAT-based interactions.
Courtesy of Drs. Leanne Hirshfield and Sidney D'Mello.

WAY AHEAD

Dr. Palazzolo is coordinating the research with ARL's Human–Autonomous Teaming Essential Research Program (HAT ERP) and Strengthening Teamwork for Robust Operations in Novel Groups Collaborative Research Alliance (STRONG CRA). Also, he shared this work with basic research counterparts at the Navy and Air Force Research Labs for Tri-Service coordination on the development of models to enhance cognitive resilience of Warfighters as a function of the teams in which they are embedded.

In addition to the government coordination of this research, Dr. Hirshfield takes a leading role in Tri-Service coordination through her Air Force Office of Scientific Research (AFOSR) grant, where she is mutually integrating this Army research with her research on the Pilot Training Next project, in collaboration with the Naval Air Systems Command (NAVAIR) and U.S. Air Force Academy. Furthermore, she has a lead role in Dr. D'Mello's new (September 2020) five-year National Science Foundation (NSF)-funded AI Institute on Student AI Teaming, which is influenced by this Army research, with similar efforts underway to develop theoretical frameworks, test beds, and metrics, in order to ultimately develop AI systems for student–AI teaming. Dr. Hirshfield will continue to collaboratively integrate and leverage the research under all these funding lines to rapidly advance her theoretical framework for swift trust and cognitive resilience in HATs.

This success was made possible by:

Dr. Edward T. Palazzolo,
Network Sciences Branch

Citations:

Eletreby, R., Zhuang, Y., Carley, K. M., Yağan, O. & Poor, H. V. *Proc. Natl Acad. Sci. USA* **117**, 5664-5670 (2020).

Tucker, P. "Special Report: The Problem with Coronavirus Models Is How We Talk About Them," Defense One. (2020).

SUCCESS STORY

Network Propagation Model Predicts Both Information and Viral Spread

This ARO initiative led to the creation of an information propagation model based on multiple strains of transmission that better predicts how information (and misinformation) campaigns evolve over time through intentional content modification as information mutates during transmission in complex networks of networks. This novel computational social science model focused on information propagation with mutations is now being used to understand COVID-19 viral mutation spreads.

CHALLENGE

Early information diffusion models focused on distributing a message throughout a network and measuring message adoption as the model's impact. However, such models fail to take into account (1) the decision-making processes of the potential adopter and (2) the ways a message changes as it moves from person to person (think of the "telephone game"). Therefore, a paradigm shift from diffusion to contagion is needed. The scientific challenges for such a paradigm shift lie in the ability to (1) mathematically define the contagion space with multiple network layers and a multistage representation of opinions, (2) computationally model information propagation while capturing evolutionary processes based on mutations of the information across large social media networks, and (3) validate the computational model with real-world data.

ACTION

Realizing that these challenges required a unique skill set, Dr. Palazzolo reached out beyond social scientists to experts in electrical and computer engineering (ECE) who were more likely to have the necessary skills to do the mathematical modeling necessary to overcome the significant challenges noted previously, but who also have the training necessary to understand the human dimension needed for modeling cognitive processes in social systems. Dr. Palazzolo identified Dr. Osman Yağan, Associate Research Professor, Department of Electrical and Computer Engineering at Carnegie Mellon University, as just such an expert. They met in person at the 2017 NetSci Conference in Indianapolis, Indiana, to iron out some of the details of Dr. Yağan's proposal, co-authored with Dr. Vincent Poor, Professor of Electrical Engineering and Dean of Engineering and Applied Sciences at Princeton University.

Drs. Yağan and Poor's proposal focused on the possibility of leveraging the classic public health epidemiological Susceptible, Infected, and Recovered (SIR) model as applied to social media information diffusion models, and extend it to a multi-network model, while capturing message mutations as the idea propagates through and across networks. From the SIR perspective, people (nodes) in a network would be coded as susceptible (S) if they have not been exposed to the message, infected (I) if they are both aware of the message and are spreading it to their contacts, and recovered (R) if they are no longer spreading the message to their networks. This expanded model is critical to understanding influence propagation in the multiplex networks as opposed to just information dissemination across a single network. For example,

Figure 3 shows the ways people connect via three simplex networks (in person, on Twitter, and via Instagram), which can be compressed into a singular, multiplex representation. Satisfied with this team's ability to address the critical information mutation problem and bolstered by the external reviews of the work, Dr. Palazzolo initiated a three-year grant in September 2017 to cover this basic research.

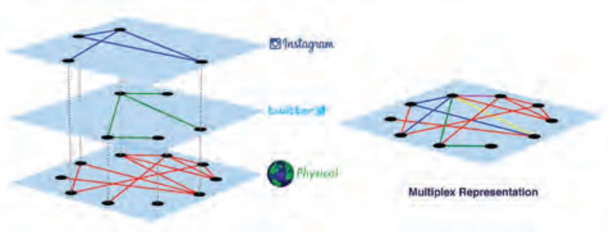

Figure 3: Left: Multi-layer network model consisting of three layers: physical layer (i.e., face-to-face interactions), Twitter, and Instagram. Vertical dashed lines connect nodes that represent the same individual. Right: Equivalent representation as a multiplex network, where links can be of different types (or colors). Since people can be connected in more than one network in the layered representation, the multiplex representation adds two additional colors to differentiate single and multiplex relationships between nodes. Courtesy of Dr. Osman Yağan.

RESULT

This propagation model research, which was initiated in 2017, became critical in 2020 to respond to a global pandemic. The discoveries from this research provide a better understanding of how information (and misinformation) campaigns can evolve over time through intentional content modification, and how viral spreading processes (such as COVID-19) might change course due to the inevitable emergence of new strains. This research by Drs. Yağan and Poor advanced the state of the art of mathematical and computational models that historically ignored evolutionary adaptations of information mutations on spreading processes in complex and multiplex networks, and now more closely model how contagion processes propagate and evolve in real life. Their work reveals the effects of evolutionary adaptations on spreading processes (be it the spread of information or a virus) and shows that classical models lead to incorrect predictions on the spreading dynamics when mutations are present. Figure 4 highlights such overpredictions of empirical data by classical models when compared to the novel computational model in both social media and face-to-face networks.

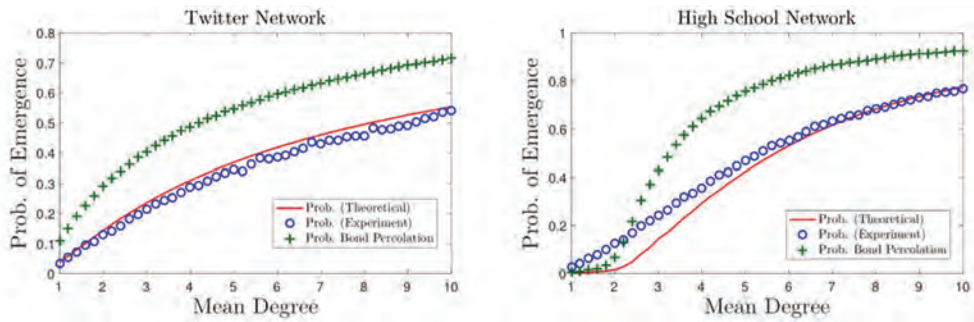

Figure 4: Two real-world contact networks: (left) Friends of 1,000 users sampled from Twitter and (right) an observed network at a U.S. high school during a typical school day. They compare the probability of the viral outbreak reaching more than 5% of the population obtained from their novel computational model (labeled theoretical) and the previous state of the art (labeled bond percolation). Adapted from Eletreby et al. (2020).

This research shows that influence spreads most effectively when hyper-influencers exist in networks where high-degree individuals (those with connections to many others in the network) tend to connect with other high-degree individuals. More specifically, these complex contagion models can be used to understand a range of social phenomena such as adoption of beliefs, norms, cultural trends, and perhaps most importantly, the rise of collective action—where social media coordination can translate to real-world activities with deleterious effects. Their work on multistage complex contagions taking place over multi-layer networks solves for the probability and expected size of large-scale cascades where the message propagation reaches a significant fraction of the population.

Building on the success of Drs. Yağan and Poor's mutation model, and the growing pandemic, Dr. Palazzolo worked with the research team to develop a rapid response grant to address two pressing needs in response to the COVID-19 pandemic: predicting mutations and predicting the impact of public health measures to reduce transmission. This new work began in Q4 of FY20.

WAY AHEAD

This new grant is expected to develop relevant findings within 12 months. Although results from this work may come too late to inform COVID-19 pandemic response planning, they will be useful for the next pandemic. The novel computational model has been shared with ARL CISD for further research on misinformation campaigns and current findings have been shared with the Walter Reed Institute of Research for consideration in their viral projections.

ARL Competencies:

- Military Information Sciences
- Humans in Complex Systems
- Network Science and Computational Sciences

Results

- Published results in the *National Academy of Science* in 2020 on the effects of evolutionaly adaptations on spreading processes in complex networks right as the global pandemic hit the United States.
- Determined that influence spreads most effectively when hyper-influencers exist in networks where high-degree individuals (those with connections to many others in the network) tend to connect with high-degree individuals.
- Discovered a model for influence propagation, now funded under a targeted COVID-19 pandemic grant to explore ability to computationally model and predict viral transmission, with the added dimension of modeling public health mitigation practices such as stay-at-home orders and mask wearing.

Anticipated Impact

This multiple-strain information propagation model has applications for (mis)information management, tracking disinformation campaigns, and predicting the scale of such information spread. Additionally, this work has implications for epidemiologists studying community spread of viral transmissions by expanding existing models for single-strain propagation to multiple-strain propagation.

WIRELESS AND HYBRID COMMUNICATIONS NETWORKS PROGRAM

Program Manager Dr. Robert Ulman

Dr. Ulman received his B.S. from the Virginia Polytechnic Institute and State University in 1984, M.S. from Ohio State University in 1986, and Ph.D. from the University of Maryland in 1998, all in Electrical Engineering.

He came to ARO in 2000 as the Program Manager for the Wireless and Hybrid Communications Networks Program.

CURRENT SCIENTIFIC OBJECTIVES

1 | Determine the fundamental limits on the capacity and secrecy in shared wireless networks that, if successful, will enable future technologies that will maximize the use of the available spectrum in congested and contested environments while ensuring secure communications.

2 | Develop methods for timely gathering, delivering, and processing of critical battlefield information that, if successful, will enable information superiority and situational awareness for command control.

3 | Achieve reliable quantum networking capabilities that, if successful, will enable secure and accurate sensing and communication capabilities.

This success was made possible by:

Dr. Robert Ulman,
Network Sciences Branch

Dr. Derya Cansever,
Network Sciences Branch

Citations:

Hua, Y., Zhu, Q. & Sohrabi, R. Preprint: arXiv:1711.10001 (2017).

Zabir, I., Maksud, A., Sadler, B. M. & Hua, Y. 2019 *IEEE Global Communications Conference* 1-6 (2019).

SUCCESS STORY

Secure Wireless Communications Bounds Using Full-Duplex Communications

Full duplex communications allow for simultaneous transmission and reception at the same time on the same frequency, which can increase throughput or also be used to keep a message secret from an eavesdropper by jamming their receiver. This research has defined the secrecy regions for using full duplex for secrecy.

CHALLENGE

Full duplex, simultaneous transmit and receive (STAR), is a concept that has been around since the 1960s; however, the amount of cancellation of transmit signal interference on the receive signal needs to be over 100 dB, which is very difficult to achieve. Recently, with advances of analog and digital signal processing, this level of cancellation has become achievable. In addition to increasing throughput, it was also recognized that full duplex could give a degree of secrecy by the intended receiver sending out a jamming signal and simultaneously receiving the desired signal by cancelling out its own known jamming signal. However, other than some heuristics such as if the eavesdropper is too close to the transmitter, the jamming will not be effective, little is known about the secrecy characteristics.

ACTION

Dr. Ulman had been following full duplex research for several years, realizing that there were two well-funded groups at Stanford University and Rice University, but was looking for research challenges beyond this hardware and system research. Dr. Ulman funded Professor Yingbo Hua at the University of California, Riverside on two Short-Term Innovative Research (STIR) grants for full duplex. Dr. Ulman realized that using full duplex for security purposes had not been well researched and this application could become a useful niche application for the Army and DoD. Therefore, in the discussion of a possible three-year grant in the area of full duplex, Dr. Ulman suggested that Professor Hua research the security aspects of full duplex communications. The resulting proposal was funded in 2017.

RESULT

Professor Hua's research resulted in several significant findings. Consider that Alice (transmitter) wants to send a message to Bob (receiver) who is using his full duplex capability to transmit a jamming signal to thwart Eve (eavesdropper) from overhearing the message from Alice. The first result is regions of locations of Eve where positive secrecy is possible as a function of the distances between Alice, Bob, and Eve, as well as Bob's ability to cancel his jamming signal in order to "hear" Alice's message (Figure 1). In addition, an algorithm to calculate the expected secrecy capacity as a function of location has been developed.

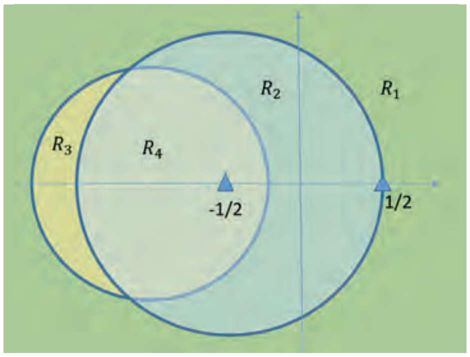

Figure 1: Regions of security. Alice is at -½ and Bob is located at ½ (distance normalized to 1). Region 1 (R_1): positive secrecy rate without jamming, but rate increased by jamming; region 2 (R_2): positive secrecy rate with jamming above a threshold; region 3 (R_3): positive secrecy for all jamming, but optimal is no jamming; and region 4 (R_4): too close to Alice, so jamming cannot create a positive secrecy capacity. Adapted from Hua et al. (2017).

A second key finding is if Eve has multiple non-collated antennas colluding, the secrecy rate rapidly goes to zero. A new algorithm, anti-eavesdropping channel estimation (ANECE), exploits the unique capability of full duplex radio to allow users themselves to estimate the channel state information (CSI) between Alice and Bob but at the same time prevent any Eve from obtaining its CSI. ANECE combines full duplex with novel designs of pilots for channel estimation. With ANECE, there is always a positive secrecy against Eve with any number of antennas. Furthermore, this work was extended to Alice and Bob also having multiple antennas (multiple-input and multiple-output [MIMO]) and with a large secrecy performance gain, when the output power was optimized for the worst-case location of Eve.

A third key finding builds upon this research, but does not require full duplex communications. Instead, it relies on CSI between Alice and Bob. There have been previous research results on this, but the secrecy was bounded by the entropy of the user's CSI. This new method, randomized reciprocal channel modulation (RRCM), is not bounded by the CSI entropy. This algorithm has been extended to include multiple antennas on Alice and Bob.

WAY AHEAD

Portions of the research have already been performed in collaboration with ARL, including joint papers with Dr. Brian Sadler. This collaboration will continue to further the research, particularly the newest results that do not require full duplex. Transition opportunities will also be pursued with other ARL cybersecurity scientists.

SUCCESS STORY

Distributed Data Processing and Machine Learning Algorithms for Wireless Battlefield Networks

A new algorithm has been developed to significantly reduce the latency of packets for real-time surveillance and control, as well as distributed fog computing.

CHALLENGE

Computing near the tactical edge of the network, where the sensors are located, will allow for a faster information processing and decision cycle, allowing Warfighters to act more quickly and decisively. To do this, small processors, wirelessly connected, will have to pass large amounts of data to move it among processors with low delay. Unlike large servers with individual wired connections between processors, the data must be passed in a congested and contested wireless environment, which leads to intermittent connectivity and mobility, changing the network topology. In addition, individual nodes have limited computational capability and limited power, requiring distributed processing. Therefore, there is a need for algorithms to get the right data to the right place within stringent delay constraints. Up until recently, most wireless network research has focused on long-term throughput as opposed to delay constraints.

ARL Competencies:

- Military Information Sciences
- Humans in Complex Systems
- Network Science and Computational Sciences

Results

- Led to a co-publication between ARL and academic researchers in the 2019 IEEE Global Communications Conference.

Anticipated Impact

New cybersecurity protocols will be further designed and deployed to enable secured wireless communications.

This success was made possible by:

Dr. Robert Ulman,
Network Sciences Branch

Dr. Derya Cansever,
Network Sciences Branch

Citations:

Tsanikidis, C. & Ghaderi, J. Preprint: arXiv:2001.05146 (2020).

ARL Competencies:

Network Science and Computational Sciences

Results

- Developed algorithms that significantly outperform the current LDF policy, improving the delivery ratio by up to 15%.
- Received the Best Paper Award at IEEE INFOCOM 2020 for "On the Power of Randomization for Scheduling Real-Time Traffic in Wireless Networks."

Anticipated Impact

This new algorithm will improve the percentage of packets delivered within delay guarantees that will facilitate real-time surveillance, augmented and virtual reality, and low-latency fog computing.

ACTION

Dr. Ulman met Professor Javad Ghaderi when he was a soon-to-graduate Ph.D. student working on a Multidisciplinary University Research Initiative (MURI) investigating medium access control with conflict graphs. When Professor Ghaderi took a position at Columbia University, Dr. Ulman recognized the potential of the research performed under the MURI, and the two worked together with Professor R. Srikant of the University of Illinois, Dr. Ghaderi's former Ph.D. advisor, to formulate a proposal. This proposal resulted in a successful grant that ended in 2019.

Dr. Derya Cansever, acting Program Manager at the time this grant ended, realized the need for new low-latency communications within a wireless environment for fog/edge computing and that the approaches of Professors Ghaderi and Srikant could potentially improve the performance of previous, more simplistic approaches. Based on discussions of this topic, Dr. Cansever suggested that Professors Ghaderi and Srikant develop a proposal, based on their grant's research but directed more toward the application of edge/fog computing, where the traffic is under delay constraints. The resulting proposal was funded in 2019.

RESULT

A multi-hop network wireless network is analyzed, similar to many tactical networks with single-link traffic with arrival deadlines. The objective is to guarantee that at least a certain fraction of packets of each link is delivered within their deadlines, which is referred to as the delivery ratio. Recently, there have been two approaches for providing quality-of-service guarantees for real-time traffic in wireless networks. One is a frame-based approach and the other is a greedy scheduling approach like the largest-deficit-first (LDF) policy. Both of these approaches have issues: the frame-based approach assumes all packets arrive before the start of the frame in order to schedule and LDF algorithms show poor performance for general traffic patterns. Building on previous research, utilizing interference graphs and randomized scheduling, Professors Ghaderi and Srikant developed a new algorithm that improves the delivery ratio guarantees for both fully connected and general wireless networks.

For fully connected networks, in addition to considering the packet deadlines in scheduling, the algorithm considers the deficit that each queue has, which represents how the queue is doing with respect to the minimum packet successful delivery ratio for the service (such as real-time video) to operate. With these two criteria, a list of queues with worst-case combinations of soonest deadlines and deficits is made and a probabilistic scheduling algorithm is used to pick the next packet to be sent. For more general networks, where there are multiple links that can be active at the same time, a similar algorithm is used for the maximal sets of non-interfering links, which leverage the interference graph results of a previous ARO grant. The resulting algorithms significantly outperform the LDF policy, improving the delivery ratio by up to 15%.

WAY AHEAD

Professors Ghaderi and Srikant are working to extend this research to multi-hop networks to include both routing and scheduling, which will be applicable to tactical mobile ad hoc networks. Also, these results will be combined with other results in predictive packet delivery that can be used in wireless augmented or virtual reality.

I S D Information Sciences Division

Computing Sciences Branch | Mathematical Sciences Branch | Network Sciences Branch | **Technology Integration and Outreach Branch**

ARMY SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM

Program Manager
Mr. Michael Caccuitto
Chief, Technology Integration and Outreach Branch

Mr. Caccuitto is a graduate of the University of Rochester, receiving a B.S. in Optics in 1991. He also received a master's degree in Business Management from Rensselaer Polytechnic Institute in 1994 and a master's degree in Public Policy from the Harvard Kennedy School of Government in 1999.

Prior to joining ARO in 2009, Mr. Caccuitto worked for almost a decade in the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics overseeing the Small Business Innovation Research (SBIR) and STTR programs, and before that, supporting various Industrial Policy initiatives. He began his career as an Air Force research, development, and acquisition officer, retiring from the Air Force Reserve in 2017.

CURRENT SCIENTIFIC OBJECTIVES

1. Align Army STTR investment portfolios with the U.S. Army Futures Command (AFC) Modernization Priorities and Cross-Functional Teams (CFTs) that, if successful, will support previously identified science and technology (S&T) needs and other AFC mission areas, including those associated with the U.S. Army Special Operations Command (SOCOM).

2. Shorten the life cycle of military technology development via a special topics pilot program using 10 Army STTR-selected projects that, if successful, will address military technology gaps for prototyping.

SUCCESS STORY
Laser-Activated Plasma (LAPLAS) for Standoff Electronic Denial

The Advanced Systems & Technologies, Inc. (AS&T) and University of Maryland (UMD) team has introduced an innovative ultra-short laser pulse technique, which when focused in air or on a target, ignites a confined burst of plasma generating broadband radio frequency (RF) radiation. Adjusting the time sequence of the laser pulse train enables the generation of a frequency-tunable RF signal of an intensity sufficient to disrupt the performance of electronic receivers operating within the same frequency band, which has direct applications for denying, disrupting, or destroying electronics onboard remote targets such as unmanned aerial vehicles (UAVs) or unmanned ground vehicles (UGVs).

CHALLENGE

Targeted generation of RF radiation has direct applications for electronic jamming of UAVs, UGVs, and other systems whose operation is dependent upon global positioning system (GPS) communication. To be effective, the jamming frequencies should be within the frequency band of the transmitter–receiver link, which for GPS communication fits one of the established L-bands. In the case of the laser-based directed-energy standoff electronic denial system, this capability requires addressing two critical problems:

1. Matching the repetition pulse rate of the laser pulse train to that of the carrier frequencies of commercial GPS systems. Thus, it is advantageous to have a tunable laser pulse rate in order to generate laser-induced RF frequencies within these same bands that may be used by a potential adversary.

2. Having each pulse in the train be of sub-nanosecond length and preferably adjustable too, as the length defines the bandwidth of the RF radiation.

This success was made possible by:

Mr. Michael Caccuitto, Technology Integration and Outreach Branch

Dr. Michael Gerhold, Electronics Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

Citations:

Jaspar, M. "Army Awards 10 Prototyping Contracts Under Small Business Pilot Program," *Nextgov*. (2020).

ARL Competencies:

Network Science and Computational Sciences

Results

- Developed a patent application to be submitted by AS&T (in process) for "Method and system for generating laser pulse train with controlled pulse rate within the sequence" (working title).
- Developed a patent application to be submitted by the AS&T-UMD team (in process) for "Method and System for frequency-tunable laser induced broadband RF radiation" (working title).

Anticipated Impact

AS&T is expected to enable future leap-ahead technologies, such as directed-energy beam control and optically broadband visual infrared countermeasures.

ACTION AND RESULT

The ARO Army STTR Program allowed each Phase I performer to provide a presentation of Phase I results and preview of their potential Phase II effort to ARL subject-matter experts and technical experts from the operational community.

In the Phase I program, AS&T proposed an alternative technology with its counter-UAV (C-UAV) denial enactment based on the use of laser-induced broadband RF radiation. It did so by performing a feasibility study of its proposed C-UAV concept and established the laser-activated plasma (LAPLAS) concept of operation and specification. The feasibility study included modeling, simulation, and laboratory validation of the LAPLAS breadboard.

The results of this work were realized through a novel configuration of a mode-locked laser capable of generating a laser pulse train with a controlled pulse separation time within the train. For this design, the team used a multi-element cavity configuration for selection of the longitudinal modes to enable generation of a single laser pulse on the period of the train (Figure 1). By aligning (or tuning) the mutual position of these elements, it was demonstrated the possibility to lase the pulse train with a controlled pulse separation time.

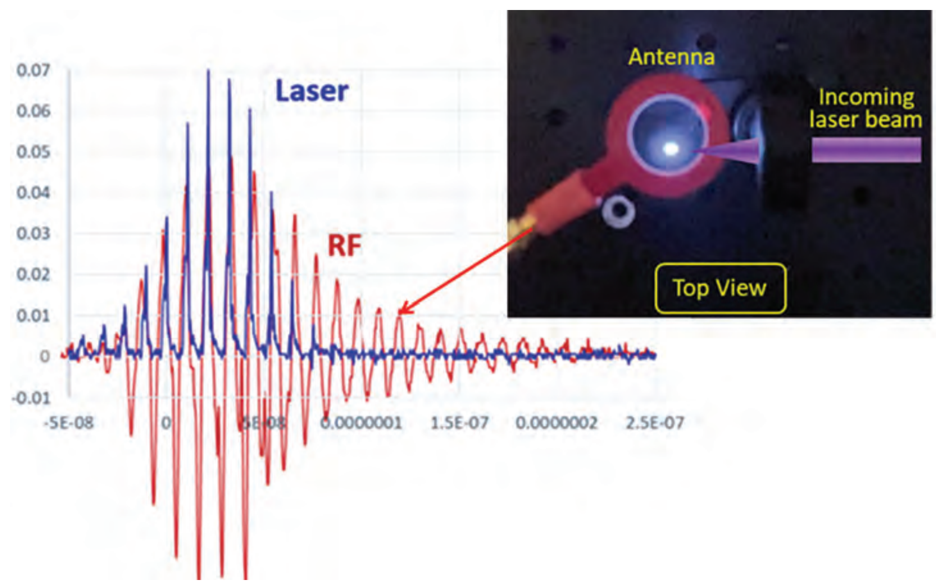

Figure 1: (Right) Schematic of the detection of the LAPLAS. (Left) The dynamic of the laser pulse train (blue) and corresponding RF signal (red). Courtesy of Advanced Systems & Technologies, Inc.

WAY AHEAD

The AS&T-UMD research team will next extend modeling of the controlled pulse train (CPT) laser and its operation, specifically the length of the pulse train envelope, duration of the individual pulse in the train, and pulse repetition rate. The next objective in this effort is to design, integrate, and validate the performance of the CPT laser and associated broadband RF radiation in the frequency bands of interest to be completed through a STTR Phase II effort. The AS&T-UMD research team will then demonstrate distant electronic denial operations in the field against various objects that are relevant to the Army and other DoD agencies. Of particular interest would be to evaluate other applications of adapted CPT laser systems, such as optical countermeasures, controlled high-voltage discharges, remote sensing, and distant pathogen detection.

SUCCESS STORY

Nonlinear RF Interference Mitigation Achieves Initial Success

In a Phase I STTR program, GIRD Systems, Inc. (GIRD), and their partner organization, the Georgia Institute of Technology (Georgia Tech), demonstrated use of its patented nonlinear analog signal processor to mitigate high-power narrow- and broadband jamming in a receiver by greater than 40 dB. The results dramatically improve the robustness of all Army radio receivers in congested/contested RF environments.

CHALLENGE

The primary challenge of jamming resistance is providing mitigation of high-power, broadband on-channel interference without an interference reference signal or knowledge of the signal of interest, while leaving the signal of interest undistorted. Interference that exhibits amplitude agility also presents a challenge for circuit-based interference solutions.

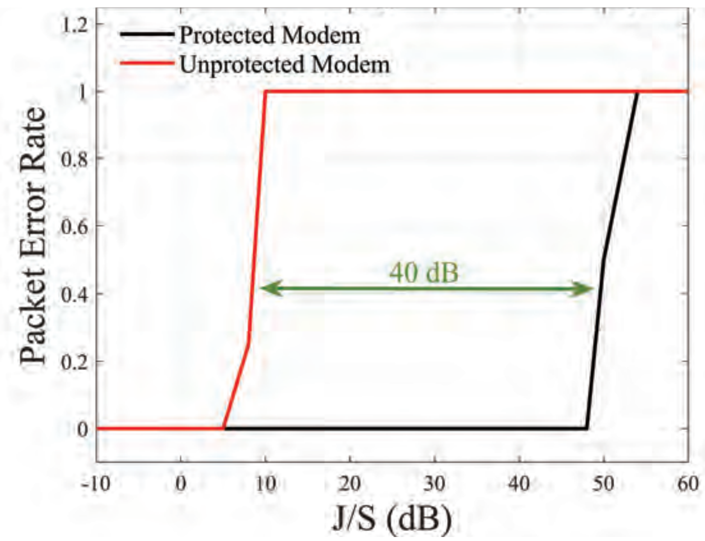

Figure 2: Headroom improvement with the initial prototype of GIRD's interference mitigation technology. Courtesy of GIRD.

ACTION AND RESULT

The Army STTR Program allowed each Phase I performer to provide a presentation of Phase I results and preview of their potential Phase II effort to both ARL subject-matter experts and technical experts from the operational community.

GIRD's novel interference mitigation solution relies on nonlinear processing to significantly reduce on-channel interference without the need for a reference signal and is agnostic to the signal of interest as well as the interference signal type (Figure 2). This enables operation as an external appliqué to mitigate RF interference in front of the protected radio or can be integrated into the RF front end. A software implementation is also available for low dynamic range conditions. While the initial demonstration targeted constant-envelope interference, a novel loop filter was also designed to track and mitigate agile-amplitude interference. The resulting technology enables applications such as communications through barrage jamming, mitigation of co-site interference, and covert communications where radio transmissions use the local RF environment to hide communication transmissions.

WAY AHEAD

The GIRD–Georgia Tech team will develop advanced prototypes using gallium nitride devices to increase the power-handling capability and the small-signal sensitivity of the nonlinear interference mitigation signal processor. A final prototype will be demonstrated at completion of the 18-month STTR Phase II program.

This success was made possible by:

Mr. Michael Caccuitto, Technology Integration and Outreach Branch

Dr. Joe Qiu, Electronics Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

Citations:

"Army selects nine small businesses, research institutes to develop prototypes," *DEVCOM ARL Public Affairs.* (2020).

ARL Competencies:

Network Science and Computational Sciences

Results

- Successfully demonstrated the initial prototype and was selected for Phase II of the STTR program.
- Led to a partnership with the Georgia Tech device team for further prototype advancement in Phase II.

Anticipated Impact

GIRD's nonlinear interference mitigation solution protects HF, VHF, and UHF receivers, and enhances operation in contested and congested environments. The solution is complementary to other interference mitigation techniques to enable a complete solution to interference mitigation in high dynamic range interference environments. The solution helps extend the operational efficacy of legacy military communications systems, while also providing another available interference mitigation tool for new systems.

ARO IN THE NEWS

Army fields new chemical detection technology

BY U.S. ARMY CCDC ARMY RESEARCH LABORATORY PUBLIC AFFAIRS | SEPTEMBER 8, 2020

Research through the U.S. Army Small Business Technology Transfer program, results in a product to accurately detect chemical weapons at low concentration levels. It is now being used by National Guard units throughout every state in the country, and the Army has begun fielding it to all units in areas where there is a threat of chemical agents. (U.S. Army).

Chemical weapons pose a serious threat to civilian and warfighter lives, but technology from the U.S. Army Small Business Technology Transfer program reduces those risks. Researchers developed a product to detect chemical weapons accurately at low concentration levels.

Active Army, Reserve and National Guard units started to receive the Chemical Agent Disclosure Spray and the Contamination Indicator/Decontamination Assurance System, known as CIDAS. The Army is fielding it to all units in areas where there is a threat of chemical agents.

The Chemical Agent Disclosure Spray, purchased by FLIR Systems, Inc., has transitioned into the CIDAS Program of Record within the Joint Program Executive Office for CBRN Defense. The research, which began 20 years ago with a business first spun out of the University of Pittsburgh and later acquired by FLIR, as part of a Small Business Technology Transfer contract managed by the Army Research Office.

ARO is an element of the U.S. Army Combat Capabilities Development Command Army Research Laboratory.

The Army funded the basic research behind this technology at the University of Pittsburgh led by Dr. Alan Russell. Russell worked to identify ways to incorporate enzymes into polymers that would be stabilized for use outside the cell and then ultimately used in realistic battlefield environments.

Typically enzymes are not stable outside the living organism, but Russell's fundamental polymer and enzyme chemistry research identified a way to maintain high activity of the enzymes for sensing chemicals in realistic battlefield conditions. He then started a small business based on those findings, which FLIR purchased.

"Our ability to respond to chemical warfare is a national security challenge that is vital to protecting both civilian and military lives," said Dr. Stephen Lee, senior scientist at the ARO. "This technology is highly sensitive, providing accurate results on only trace amounts of material, even at concentrations below levels that represent an immediate danger to life and health."

The new technology uses enzymes (complex proteins naturally produced by living organisms that act as a catalyst for specific biochemical reactions) to drive rapid, color-based reactions with chemical warfare agents. Once applied to a surface as a liquid solution, a vivid color change indicates the exact location of contamination by a specific chemical warfare agent.

Because the underlying chemistry uses enzymes to drive specific biochemical reactions, the technology is highly resistant to potential forms of chemical and environmental interference that might be problematic for conventional detection equipment.

The product's sensitivity also provides the ability to determine whether decontamination was effective.

"Our Agentase C2 spray technology offers unprecedented performance, enabling rapid detection of highly toxic substances while reducing the lifecycle cost of decontamination operations," said David Cullin, vice president of business development-Detection for FLIR Systems.

Products previously available for the detection of nerve and blister chemical agents range from simple units that use colorimetric techniques, wherein the presence of a chemical substance is indicated by a specific color change, to more complex systems that use special equipment.

Unfortunately, most colorimetric-based products such as paper detection products or gas detection tubes, can be highly susceptible to chemical interference, which can result in false positive and false negative results, as well as poor sensitivity.

> **"Through the Army's Small Business Technology Transfer program, a small business has changed our nation's ability to respond to chemical attacks," Lee said. "The Army is taking advantage of the latest breakthroughs in synthetic biology to field new capability and protect national security. Without that program, we'd never have the ability to field this capability."**

The STTR program funds research and technology development with small businesses working in partnership with research institutions, most often colleges or universities. In contrast to the basic research programs managed by ARO, the STTR program focuses primarily on feasibility studies leading to prototype demonstration of technology for specific applications.

The Defense Threat Reduction Agency, the DOD agency responsible for countering weapons of mass destruction, provided additional funding to bridge the technology from development to capability delivery.

JPEO-CBRND, the DOD entity that manages the nation's investments in chemical, biological, radiological and nuclear defense equipment, adopted the technology as part of the Domestic Response Capability Kit.

The kit packages the chemical components into a simple, pen-like construct, an easy-to-use point-and-touch detection as well as a spray-based formulation of the same technology. The kits have been fielded to all 57 Army National Guard Weapons of Mass Destruction Civil Support Teams across the country.

Now, National Guard units throughout every state maintain the capability to provide for detection, personal protection, decontamination and medical monitoring against chemical agents.

Additionally, JPEO-CBRND recently awarded FLIR an indefinite-delivery/indefinite-quantity five-year contract worth up to $21.8 million to support the Army's Contamination Indicator/Decontamination Assurance System program.

This award initiates the full-rate production phase to field the product to units throughout the Army. Shipments are expected to begin in the fourth quarter of 2020.

Senior Research Scientist Spotlight | Dr. Stephen J. Lee
Senior Research Scientist, Interdisciplinary Sciences, ARO

Dr. Lee completed his undergraduate studies at Millsaps College, receiving his B.S. in Biology and Chemistry in 1991. He trained as a physical organic chemist at Emory University, receiving his Ph.D. in Physical Organic Chemistry in 1996.

He came to ARO in 1998 as the Program Manager for what was then called the Organic and Inorganic Chemistry Program. In 2007, he became an Army corporate ST in the Executive Service, spending time serving as the ARL Chief Scientist and the ARO Chief Scientist.

Dr. Lee is the ARO Senior Research Scientist for Interdisciplinary Sciences, which includes planning and developing the future vision of basic research for ARO while maintaining an active research program. His work at ARO includes basic research directed toward hazardous materials management, including studies in decontamination, detection, and protection. His awards include the Presidential Rank Award, the Theodore Roosevelt Government Leadership Award, and the Top Outstanding Young American Award.

As mentioned, Dr. Lee's main research focus at ARO is directed toward hazardous materials management, including studies in decontamination, detection, and protection. As such, Dr. Lee is involved in the fielding and transition of many technologies and capabilities to the Soldier, including decontaminants, detectors and sensors, field protection equipment, and general gear. One particular topic he has been involved in for a number of years is the coordination and management of research programs in the Army focused on basic and applied research needs for military working dogs.

Fully fielded in 2020, the Chemical Agent Disclosure Spray and the Contamination Indicator and Decontamination Assurance System (CIDAS) research is an excellent example of an ARO basic research breakthrough leading to a revolutionary new capability for the Soldier. This research, supported initially at the University of Pittsburgh by the Reactive Chemical Systems Program in the Chemical Sciences Branch demonstrates the contribution and impact that academic basic research can have toward fielding a new military capability. The original work of Professor Alan Russell, now Vice President of Biologics at Amgen Inc., was to stabilize specific enzymes and proteins outside living organisms, while maintaining their chemical activity when exposed to battlefield environments and temperature ranges from below freezing to over 120 °F. While initially studying enzymes that could break down and destroy chemical warfare agents, Professor Russell discovered a unique way to detect chemical warfare agents.

Professor Russell's research tested the hypothesis that enzymes could be stabilized outside of living organisms by encapsulating them in polymers that would maintain reactivity and, in fact, extend the reactivity and lifetime of the enzymes. Professor Russell focused on how the enzymes of interest could be modified to react in polymerization without being denatured. The breakthrough originally indicated that he could stabilize enzymes through polymerization, and this led to the development of a "living" combination of enzymes that could be used to detect chemical warfare agents with great specificity and stability. The "living" enzyme system can detect chemical warfare agents at the tens of molecules of agent and was thus incredibly more sensitive than any system the Army fielded. Using enzymes for detection is not new, but Professor Russell's work lead to being able to take the capability to the field without needing a whole laboratory of support.

ARO utilized the Small Business Technology Transfer (STTR) program as a mechanism to transition the fundamental scientific discovery to Agentase, a small business established to refine and package the synthetic biology. Professor Russell, in collaboration with Dr. Keith LeJeune, founded Agentase, LLC, to take the basic research discovery to a fieldable sensor. The STTR program funded the development of the form factor for fielding and supported in-depth real agent testing proving the effectiveness of the "living" chemical warfare agent detection system. The success in the first STTR effort led to a subsequently-phased STTR efforts to facilitate the acquisition process, and eventually a new capability for detection. Ultimately, with successful Phase I and II efforts STTR, the subsequent Phase III efforts exceeded $50M to field the new detectors.

Agentase developed and distributed the product to a limited number of select user groups who fielded the sensor system. As the Joint Program Executive Office for Chemical and Biological Defense (JPEO-CBD) monitored the detection system's progress and capabilities, they initiated a new program of record known as the CIDAS program. Partnerships between ARO, the Defense Threat Reduction Agency (DTRA), the National Guard, and the JPEO-CBD led to the full development of the CIDAS program using the enzymatic-based systems supported and developed under ARO's basic research program. ARO's partnering with key government organizations and leveraging research, development, testing, and evaluation (RDT&E) and Army acquisition cemented this new capability for the Soldier. Dr. Lee led the technology push to create this product from an ARO basic research breakthrough with Professor Russell to today's fielded CIDAS. During the development of CIDAS, Army acquisition contributed the tools and resources required to keep the detection biology and chemistry progressing toward a new detection platform and the unique ability to verify if items were truly decontaminated and safe. As the success of the science to technology became publicized, Agentase became a part of a multinational traded company and finally to a wholly owned part of FLIR Systems. In summary, CIDAS demonstrates the value of Small Business Innovation Research (SBIR) and STTR programs to successfully develop a new sensor capability for the Soldier and create a new business that is effectively supporting national security.

ARO SMALL BUSINESS INNOVATIVE RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM

Program Manager
Ms. Nicole Fox

Ms. Fox completed her B.A. in Business Administration at Bay Path University in 1997.

She came to ARO in 2010 as a contracted Program Specialist for the Army STTR program and was promoted to a government position as the ARO SBIR/STTR Program Manager in 2011.

CURRENT SCIENTIFIC OBJECTIVES

1 | Develop strong, germane, and competitive topics to stimulate technological innovation that focus on ARL's Technical Competences and the Army's Modernization Priorities that, if successful, are anticipated to lead to breakthrough research and development (R&D) that participating small businesses and university partners can then commercialize through sales in the private sector or back to the government.

2 | Establish close ties with academia, startups, and established small businesses to achieve further insight into technology transition through funding mechanisms, program of record needs, Warfighter requirements, and Program Executive Offices (PEOs) that, if successful, are anticipated to develop methods to assist small businesses, academia, and program managers to advance the transition of their technologies to meet the needs of the Army.

This success was made possible by:

Dr. James Parker, Chemical Sciences Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

SUCCESS STORY

Low Temperature Electrochemical O_2 Pumps for Medical O_2 from Air

Global Research and Development Inc. (Global) has successfully proven the technology for using nano-layered oxygen (O_2) pumps to concentrate medical purity O_2 from ambient air. This proof of concept shows the potential to greatly improve the availability of medical-grade O_2 to Soldiers in the field and at the bedside in hospitals without the dangers of O_2 cylinders or the unreliability and purity limits of pressure swing absorption (PSA) units. The company is now positioned to transition the first lightweight, portable, plug-in or battery-operated O_2 purification technology to the commercial market and the Warfighter.

CHALLENGE

In the medical community, the size, weight, and power of current portable O_2 devices do not meet the new Army goals. The logistical complexity of supplying O_2 in large gas cylinders makes current systems cumbersome and not easily deployable, particularly to some of the contested environments of the military. The challenge is to develop a device that is able to separate O_2 from ambient air and process it into the required O_2 concentration for medical use, while maintaining the required size, weight, and power consumption the Army requires.

ACTION

In 2017 Dr. Michael Gerhold, in coordination with the Defense Health Agency (DHA), developed a STTR topic titled "Oxygen Production and Delivery on Demand." Under this topic, DHA awarded one STTR Phase I contract to Global. Upon successful completion of the Phase I contract, Global submitted a Phase II proposal with its research institution partner, Ohio State University, which was selected to continue further developing this technology. Ms. Fox served as co-contracting officer's representative (COR) with Dr. James Parker (Chemical Sciences Branch) taking over for Dr. Gerhold.

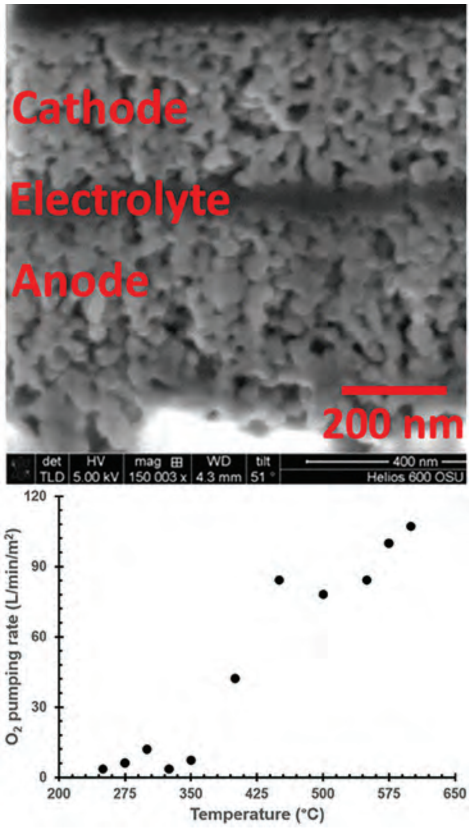

Figure 1: Scanning electron microscopy cross section of the deposited layers of an electrochemical O_2 pump atop a porous support (top) and the achieved O_2 output flowrates at the tested temperatures (bottom). Courtesy of Global Research and Development Inc.

RESULT

This STTR project resulted in the development of electrochemical O_2 pumps for use in military medical applications. These O_2 pumps use a small applied voltage to drive O_2 from ambient air across the pump's nano-layered structure to obtain high-purity (near 100%) O_2 on the permeate side (Figure 1). This concept has been proven in a flat geometry and this project will transfer the technology onto larger-scale tubular supports for more compact and practical O_2 generation systems.

Global also demonstrated the ability to fabricate porous tubular supports (14 inches long x 1 inch diameter) that are suitable in a variety of separation applications for gasses and liquids while maintaining the necessary surface microstructure of the supports. This is an important step in developing the scalability of the fabrication process to a commercial magnitude.

WAY AHEAD

To achieve reliable and competitive medical O_2 generation, Global must now optimize their individual layer thicknesses and microstructures. This will be achieved by pursuing a SBIR Phase II Enhancement to develop automated equipment to replace the human-operated manufacturing equipment.

SUCCESS STORY

Multi-Hit Performance of Small-Arms Protective Armor

The Warfighter is the most weight sensitive and highest value of all assets, and thereby utilizes the most advanced and expensive materials in their protection systems. Transparent Armor Solutions' effort under the STTR program provided a significant improvement in understanding the multi-hit behavior of boron carbide (B_4C) ceramic-based body armor and similar armor systems.

CHALLENGE

In 2016, the U.S. Army developed an $80 million program to reduce the weight of hard body armor plates by 2 lb (~20%). While this may appear like a modest amount of weight to pull out of an armor system, it is in fact extremely difficult to achieve reliably. The highest-performing and most-expensive materials are already being used for body armor and are the most difficult and expensive to improve. Barring a disruptive breakthrough in ceramic or composite materials, measurable weight reductions in body armor have proved elusive.

The difficulties associated with computational modeling of body armor are not to be underestimated. It is one of the single most difficult tasks in the armor/anti-armor community, even when compared to the multi-physics codes required for modeling shaped-charge jet formation, explosive reactive armor (ERA), and electromagnetic armor systems. The difficulty lies in the advanced materials that constitute body armor and aircraft armor, engineered ceramics, and high-strength composite materials. These materials also happen to be exceedingly difficult to characterize in quasi-static and high strain rate mechanical testing.

There are typically at least two impacts within close proximity to one another that need to be considered. Multi-hit impact further increases the complexity of the problem because one has to account for and predict the damage accumulation and extent in the

The highest-performing and most-expensive materials are already being used for body armor and are the most difficult and expensive to improve.

ARL Competencies:

Sciences of Extreme Materials

Results

- Developed functional nano-layers deposited onto tubular supports.
- Designed and fabricated laboratory processing equipment for making tubular supports and the tubular nano-layer coating.

Anticipated Impact

Global anticipates that their technology can greatly improve the availability of medical-grade O_2 to Soldiers in the field and at the bedside in hospitals without the dangers of O_2 cylinders or the unreliability and purity limits of PSA units. There is the possibility that some of the developments made in upscaling the O_2 pumps can be put into use for water filtration and electricity generation using solid-oxide fuel cells.

This success was made possible by:

Dr. David Stepp, Chief Scientist

Ms. Nicole Fox, Technology Integration and Outreach Branch

Citations:

Anderson, Jr., C. E. & Grosch, D. J. *SwRI Technical Report* 18.24210/001 (2019).

Holmquist, T. J., Chocron, S. & Nicholls, A. *SwRI Technical Report* 18.24210/003 (2020).

Holmquist, T. J. *SwRI Final Report* 18.24210/003 (2020).

Holmquist, T. J., Chocron, S. & Nicholls, A. J. *American Ceramic Society* (in review).

South, T. "Study Looks at Ongoing Army, Marine Efforts to Lighten Body Armor, Troop Load," *Army Times*. (2017).

Weiss, C. E. *SwRI Final Report* 18.24210/002 (2019).

armor system, and also account for the degradation in performance as a result of the damage for subsequent impact predictions. Because the damage accumulation has such a significant effect on the kinetic-energy absorption capability of the armor, it is imperative to characterize and quantify it for comparison to the computation predictions, as well as help inform experimental development of future armor solutions.

ACTION

In 2015 Dr. David Stepp adopted a STTR topic from DEVCOM SC titled "Multiple Hit Performance of Small Arms Protective Armor." The small business Transparent Armor Solutions, along with their research partner Southwest Research Institute (SwRI), submitted a STTR Phase II proposal that was competitively selected. B_4C, the focus in the present work, is of interest as an armor material because it is the lightest engineered armor ceramic as well as one of the hardest bulk materials (second only to diamond). This lightweight and hard ceramic serves to disrupt and break up an incoming projectile. The broken projectile can be defeated in an advanced composite back plate. However, the ceramic also undergoes significant fracture in this process. Predicting the behavior of B_4C has proved to be more exacerbating than its counterpart silicon carbide (SiC), which is also employed in body armor and rotary-wing armor systems, and was the focus in the STTR Phase I and II efforts. Ms. Fox served as co-COR with Dr. Stepp on the STTR contracts.

RESULT

This STTR project resulted in a better understanding of the multi-hit behavior of B_4C ceramic-based body armor through careful implementation of ballistic experiments and the development of computational tools for prediction of multi-hit impacts in this type of armor system.
It achieved this by developing finite element modeling (FEM) tools that allow for investigating multi-hit behavior of ceramic body armor designs computationally, a first of its kind.

The premise of this program was to understand and predict the multi-hit ballistic insult behavior of B_4C and SiC ceramics, which are typically used in body armor and rotary-wing aircraft armor applications. There were multiple research streams operating in series and parallel over the two-year effort. Phase I focused on SiC, whereas Phase II emphasized B_4C and also included ultra-high molecular weight polyethylene (UHMWPE) back plates. The high strain rate and quasi-static behavior of B_4C was characterized through a series of careful experiments along with some laboratory ballistic testing. The computational material model constants were derived from these experiments.

The 6- × 10-inch ceramic targets were scaled up from the 5- × 7-inch ceramic tile (Figure 2). The impact spacing is denoted in projectile diameters. For a 30-caliber projectile, which has an outside diameter of 0.30 inch (7.62 mm), corresponds to a spacing of 3 inches (76.2 mm) at 10 projectile diameters (10D). The areal density of the ceramic was held nominally constant for the targets accounting for the density difference between the Coors Vista SiC-N (3.20 g cm^{-3}) and pressure-assisted densification (PAD) B_4C (2.49 g cm^{-3}) and using a B_4C tile that was approximately 23% thicker than the SiC-N used in the Phase I/Phase II effort.
A typical simulation result for B_4C is shown in Figure 3.

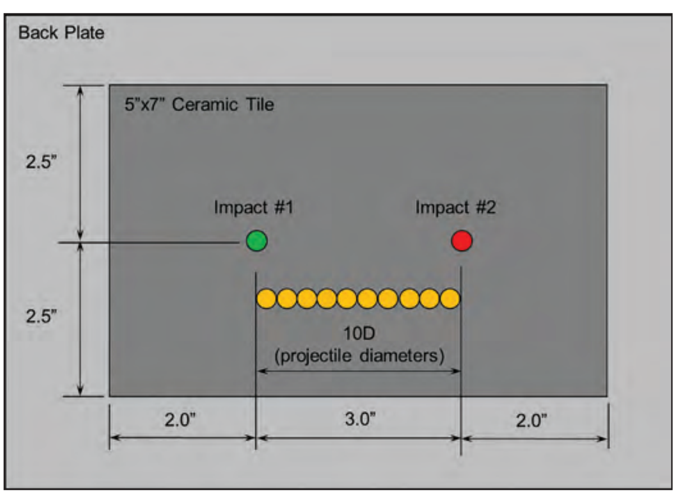

Figure 2: Example of a 5- × 7-inch ceramic tile target showing the impact locations for 10D spacing of a 30-caliber projectile. Courtesy of Transparent Armor Solutions, SwRI, University of California, Los Angeles (UCLA).

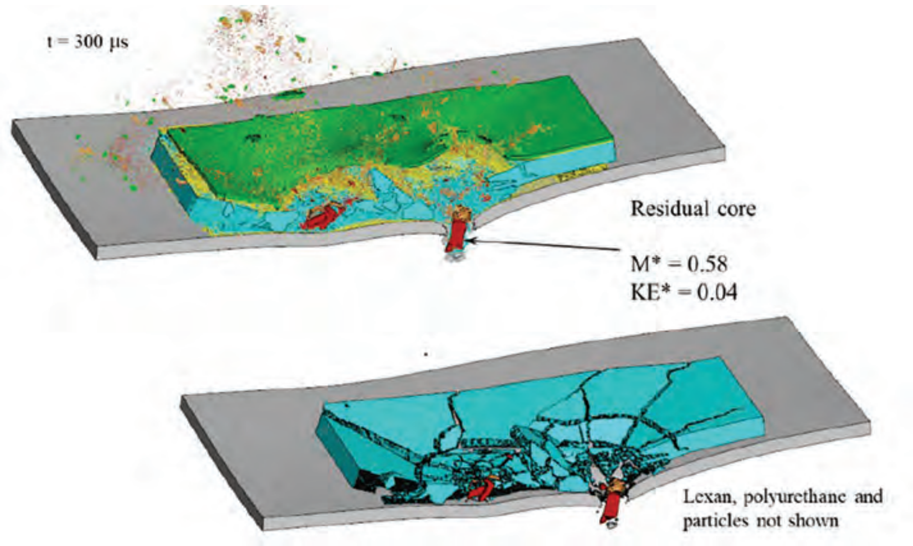

Figure 3: Computation of a 5- × 7-inch B_4C ceramic tile target being impacted by two sequential impacts spaced 8 projectile diameters apart. The first impact was stopped while the second impact, in the damage zone of the first impact, perforates the target. The bottom image shows the ceramic without smoothed-particle hydrodynamics (SPH) particles and the polycarbonate cover to illustrate the computed damage. Courtesy of Transparent Armor Solutions, SwRI, UCLA.

WAY AHEAD

This work will aid in the requirements of the PEO community in understanding the implications of new weapon systems; ammunition; training, tactics and procedures (TTPs); and equipment requirements. The intent is to utilize this suite of tools to supplement mechanistic information we are unable to obtain from advanced ballistic experiments.

ARL Competencies:

Sciences of Extreme Materials

Weapons Sciences

Results

- Resulted in four technical reports from SwRI and one peer-reviewed publication in the *Journal of the American Ceramic Society* (pending review).

Anticipated Impact

This work will lead to the discovery of new mechanisms to improve the efficacy of the current state of the art in ceramic armor systems and provide direction for future material development.

EDUCATION OUTREACH PROGRAM

Program Manager
Ms. Jennifer Ardouin

Ms. Ardouin completed her B.S. in Psychology at the University of Maryland, European Division, Heidelberg, Germany, in 1991 and earned an M.S. in Industrial and Organizational Psychology from Capella University in 2004. Ms. Ardouin pursued her career interests through active duty U.S. Army service, and state and federal government service.

She came to ARO in 2017 as Manager of the Army's High School Apprenticeship Program (HSAP), the Undergraduate Research Apprenticeship Program (URAP), and various other science, technology, engineering, and mathematics (STEM) outreach activities.

CURRENT SCIENTIFIC OBJECTIVES

1. Introduce students to the Army's interest and investment in science and engineering research through associated educational outreach efforts to support preparing students for the 21st century workforce.
2. Provide hands-on research experience for high school and undergraduate students through Army-funded apprenticeships anticipated to lead to student career exploration and promote interest in STEM fields of study.
3. Grow the scale of high-quality mentorship experiences for students who would benefit from the expertise of world-class scientists and engineers as mentors for professional and academic development.
4. Coordinate selection of and engagement with National Defense Science and Engineering Graduate (NDSEG) Fellows that, if successful, has the capability to maximize potential contribution to the defense research ecosystem.

This success was made possible by:

Ms. Jennifer Ardouin, Technology Integration and Outreach Branch

Citations:

"Student Research Internships and Apprenticeships," *Hopkins Extreme Materials Institute (HEMI), Johns Hopkins University*. (2020).

SUCCESS STORY
Ensuring Summer Apprenticeship Programs in the Midst of COVID-19 Restrictions

Approximately 90% of the HSAP and URAP appointments were converted to virtual opportunities for 2020 due to the onset of the global COVID-19 pandemic.

CHALLENGE

In March 2020, just as student applications were due for the HSAP and URAP opportunities available for 2020, the global COVID-19 pandemic escalated, causing universities and high schools to transition to a virtual landscape for teaching and research. This put into question whether universities would, for the first time, have the infrastructure to safely host meaningful apprenticeships using a virtual environment. Given the importance of HSAP and URAP in exposing promising high school and undergraduate students to STEM opportunities and university-structured research environments, Ms. Ardouin, the ARO Education Outreach Program Manager, wanted to find a way to ensure these experiences could be transitioned to a virtual landscape.

ACTION

The first step in modifying the HSAP and URAP summer appointments during COVID-19 was to ensure ARL approved of the transition to a virtual environment, rather than postponing or cancelling the 2020 session altogether. Ms. Ardouin, along with her partners at the Army Educational Outreach Program (AEOP), rapidly developed a procedure that the virtual apprenticeships would

Given the importance of HSAP and URAP in exposing promising high school and undergraduate students to STEM opportunities and university-structured research environments, Ms. Ardouin, the ARO Education Outreach Program Manager, wanted to find a way to ensure these experiences could be transitioned to a virtual landscape.

follow that was swiftly approved by ARL. The new procedure required that principal investigators who had submitted an HSAP/URAP proposal modify their project plan to fully outline a virtual or hybrid plan of action for HSAP and URAP awardees. Proposals that remained onsite or were a mix of onsite and virtual had to contain detailed safety measured for students and staff. Ms. Ardouin reviewed each modified proposal and consulted the ARO Program Managers with the required technical expertise to ensure that the proposed safety guidelines and research objectives would be feasible in a virtual environment. She then aggregated the list of schools that were prepared to move forward with the apprenticeships and provided guidance to help each institution navigate restrictions while also maximizing value for each student's experience.

RESULT

In light of the COVID-19 pandemic, many other local, state, and federal STEM organizations were forced to postpone or cancel STEM-related internships and opportunities in 2020. For the HSAP and URAP programs, approximately 90% of the original student applicants were able to complete their apprenticeships in 2020 (i.e., 82 out of the 90 proposed apprenticeships).

Ms. Ardouin's actions highlighted the agility and commitment of the AEOP and ARO to carry out the goals set forth through both HSAP and URAP to engender significant experiences for the students and provide training opportunities in STEM fields. These efforts did not go unnoticed by the academic community, as exemplified in a recent report, "Student Research Internships and Apprenticeships" (2020), from Johns Hopkins University by Professor K. T. Ramesh, the Director of the Hopkins Extreme Materials Institute (HEMI) that noted:

> *Given the pandemic, all of our internships had to be conducted completely remotely this year. I am extremely proud of the students and the research activities they accomplished under these constrained circumstances! I am also grateful to the faculty hosts, mentors, and administrative personnel who ensured the students had the resources and received the guidance needed for a rich and rewarding experience. HEMI would like to acknowledge the following organizations who made these opportunities possible: the Army Educational Outreach Program, the DEVCOM Army Research Laboratory and Army Research Office, the National Endowment for the Arts, the Maryland Institute College of Art, and The Whiting School of Engineering at Johns Hopkins University.*

In a personal correspondence to Ms. Ardouin, Esther Bistricer, a 2020 HSAP apprentice, recently reflected on her experience at New York University (NYU), where she studied different techniques for characterizing and controlling quantum mechanics:

> *I was so privileged to participate in the 2020 HSAP program at NYU's Shabani Lab. I've been meaning to write an email to thank you for the amazing opportunity! It was incredibly valuable and something I never would've had the opportunity to do if not for AEOP. I also keep my ARO coin and certificate on display which brings me a lot of joy.*

WAY AHEAD

The quick, decisive action completed in 2020 has laid the groundwork to set HSAP and URAP up for success in 2021. With COVID-19 continuing to impact in-person apprenticeship experiences, Ms. Ardouin was able to ensure that universities looking to participate in 2021 apprenticeships submit proposals that detail how research groups can continue to host students in a meaningful way in the virtual environment. To date, 39 proposals have been submitted for FY21, ensuring that even under extraordinary circumstances, ARO's commitment to STEM does not falter.

ARL Competencies:

- Sciences of Extreme Materials
- Photonics, Electronics, and Quantum Sciences
- Military Information Sciences
- Biological and Biotechnology Sciences
- Humans in Complex Systems
- Network Science and Computational Sciences
- Terminal Effects
- Weapons Sciences
- Electromagnetic Spectrum Sciences
- Energy Sciences
- Mechanical Sciences

Results

- Enabled 90% of successful HSAP and URAP applicants to complete a summer internship in 2020 amidst the COVID-19 pandemic.
- Proved that the AEOP and ARO are agile in their ability to conduct the programs under dynamic, uncertain conditions.
- Garnered positive feedback from participants saying, via completion surveys, that they were pleased that they could still safely and effectively participate in a STEM program when so many others were cancelled.

Anticipated Impact

Students who participated in HSAP and URAP summer apprenticeships in 2020 will have a lasting favorable impression of the program and the importance of science conducted for and by the DoD.

HISTORICALLY BLACK COLLEGES AND UNIVERSITIES (HBCU) AND MINORITY-SERVING INSTITUTIONS (MI) PROGRAM

Program Manager
Ms. Patricia Huff

Ms. Huff is a graduate of Howard University, receiving her B.A. in Broadcast Management in 1987. Her professional activities and accreditations include Master Certified Facilitator and Moderator (Qualitative Researcher).

Prior to joining ARO in 2012, Ms. Huff worked for more than a decade in the federal government at the National Oceanic and Atmospheric Administration (NOAA). She went on to work as a marketing research analyst for the Potomac Electric Power Company (PEPCO) and later became the owner and chief executive officer (CEO) of a marketing and communications consulting company.

CURRENT SCIENTIFIC OBJECTIVES

1 | Expand the participation of HBCUs/MIs in ARO Core research programs through innovative outreach and program design/execution.

2 | Enhance the capacity of HBCUs/MIs to compete effectively for ARO research grants.

3 | Provide outreach and research experiences to faculty and students at HBCUs/MIs to increase awareness of Army research, partnerships, innovation, and career opportunities.

This success was made possible by:

Ms. Patricia Huff, Technology Integration and Outreach Branch

SUCCESS STORY

North Carolina Agricultural and Technical State University (NC A&T) Influence on the Materials in Extreme Dynamic Environments (MEDE) Collaborative Research Alliances (CRA)

In FY20, the last year of full ARL Partnered Research Initiative (PRI) programmatic operation, NC A&T made extraordinary advances, specifically in tailoring magnesium (Mg) alloy systems through composition/microstructure/severe plastic deformation. This project worked in collaboration with ARL and MEDE CRA members to maximize the impact of their research.

CHALLENGE

The PRI Program began in FY17 with the selection of four projects totaling $1.35M to participate in highly collaborative research through ARL's CRAs and Collaborative Technology Alliances (CTAs). CTAs and CRAs are large collaborative partnerships, focused on developing and transitioning research in Army-critical areas. The focus of the PRIs projects is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army by bringing competitively selected HBCUs/MIs research teams into existing ARL CTAs or CRAs.

A PRI awardee, NC A&T, was challenged with developing novel thermomechanical processing techniques for Mg alloy systems for advanced armor applications. Their partnership with Johns Hopkins University (JHU) as part of the MEDE CRA specifically provided NC A&T with an exciting opportunity to work collaboratively toward the development of novel Mg alloy systems for enhanced armor applications using and developing state-of-the-art thermomechanical treatments to leap ahead and meet the MEDE program's mission requirements, while enhancing the depth and breadth of NC A&T's research capacity, education, and infrastructure.

ACTION

Ms. Huff facilitated collaboration between the schools and ARL, and created opportunities to share information. This PRI is providing a critical and unique metals processing capability for the MEDE CRA that is currently not available within ARL.

Funding over these four years has created a capacity in the HBCU/MI base by creating new labs, strengthening of graduate programs, and providing other evidence of viable research capability.

RESULT

As a result of sustained and vigorous research efforts of this PRI project, the following has been accomplished by NC A&T:

1. Established a differential speed rolling (DSR) mill system to process Mg alloys for armor applications.

2. Established an electron backscattering diffraction technique for texture analysis of rolled and equal channel angular extrusion (ECAE) processed materials.

3. Added new educational modules on the properties and processing of low-symmetry alloys (e.g., Mg alloys for Army applications) to the materials science curriculum to educate and enhance workforce development.

NC A&T is also the sole supplier of customized Mg alloy chemistries to the ARL MEDE CRA. NC A&T developed a state-of-the-art melting/casting system to meet the requirement for severe plastic deformation processing studies at JHU and ARL. With NC A&T's process innovation acumen, they were able to cast high-quality Mg-aluminum, Mg-zinc (Zn), and Mg-Zn-calcium alloys for the entire consortium with respect to lightweight armor applications and other Army needs.

WAY AHEAD

NC A&T is developing deep science knowledge for the fabrication and processing of Mg materials with specific characteristics for enhanced dynamic and spall strength. At the same time, NC A&T is developing the fundamental understanding and ability to control of the concurrent processes of dynamic recrystallization/grain refinement and precipitation, as well as the texture evolution behavior of these novel alloys under different process conditions induced by differential speed rolling. These research areas will be transitioned to the MEDE CRA and ARL.

ARL Competencies:

Sciences of Extreme Materials

Results

- Developed a novel processing of Mg alloys in response to MEDE computational models that will lead to improved protection materials for military vehicle applications.
- Supported four doctoral students, three of whom are current Ph.D. candidates and one of whom graduated.
- Supported one master's of science student, who is now a Ph.D. candidate in Biomedical Engineering at NC A&T.
- Supported six undergraduate students during their research internships.
- Facilitated 8 peer-reviewed publications (journal and conference proceedings), 14 conference poster presentations, 9 conference technical presentations, and 10 conference keynote and invited presentations.

Anticipated Impact

These processed alloys from NC A&T are providing pivotal materials to the MEDE CRA to be developed for armor applications with enhanced microstructural and mechanical property characteristics to improve Solider survivability.

ELECTROCHEMISTRY PROGRAM

Program Manager
Dr. Robert Mantz

Chief, Chemical Sciences Branch

Dr. Mantz completed his undergraduate studies at the United States Air Force Academy, receiving his B.S. in Chemistry in 1989. He received his M.S. in Chemistry from California State University, Northridge in 1994 and his Ph.D. in Chemistry from North Carolina State University in 1997.

He came to ARO in 2006 as the Program Manager for Electrochemistry and was promoted to the additional role of Chief, Chemical Sciences Branch, in 2017.

Current Scientific Objectives

1 | Synthesize and characterize new electrolyte species to enable, if successful, advanced power storage and generation devices that provide greater capacity and with lower weight for the Soldier.

2 | Understand transport in heterogeneous charged environments to allow, if successful, selective control of transport of species enabling advanced sensors, protective gear, and fuel cells.

3 | Understand how material and morphology affect electron transfer and electro-catalysis to enable, if successful, synthesis, oxidation, and reduction of Army-relevant materials and energy systems.

4 | Explore new methods of controlling electrochemistry to enable, if successful, the creation of novel materials including new optical materials for rapid and resilient communication and computation capabilities for the Army network.

This success was made possible by:

Dr. Robert Mantz, Chemical Sciences Branch

SUCCESS STORY
Single-Particle Spectroelectrochemistry

Details about nanoelectrode size, shape, and assembly are essential to achieving a mechanistic model for how charges transfer in nanomaterial energy sources. ARO investment in correlated single-particle spectroelectrochemistry allowed the development of a kinetic model that is expected to provide the foundation for future lightweight energy storage devices.

CHALLENGE

Technological advances in battery technology can decrease the Soldier-borne weight for infantry in the field. The Army infantry Soldier, who typically carries a significant load, will be significantly advantaged by the development of lightweight rechargeable energy sources. Lightweight energy storage devices made from nanoscale electrodes could address this challenge, but because of their intrinsic heterogeneity, a knowledge of sub-ensemble kinetics of even simple electrochemical processes is crucial.

ACTION

Dr. Mantz recognized that understanding the physicochemical processes governing plasmonic electrode reshaping would provide a method to tune nanocatalyst shape and content, ultimately enabling new lightweight, rechargeable energy sources. Dr. Mantz actively worked with researchers to recruit white papers and proposals to fund research into single-particle electrochemistry. He facilitated a collaboration that began in 2019 between European researchers who have developed a highly specialized laser-based method for synthesizing gram quantities of alloyed nanoparticles and American researchers who have developed a highly specialized spectroelectrochemical technique to ascertain the rates of reactions of individual nanoparticles in real time. Dr. Mantz also recommended a Defense University Research Instrumentation Program (DURIP) award to the team (which was selected for funding) for an integrated scanning electrochemical and high-speed snapshot darkfield spectroscopic microscope capable of simultaneous electrochemical imaging, manipulation, and high sensitivity spectroscopy of single plasmonic nanoelectrode structures.

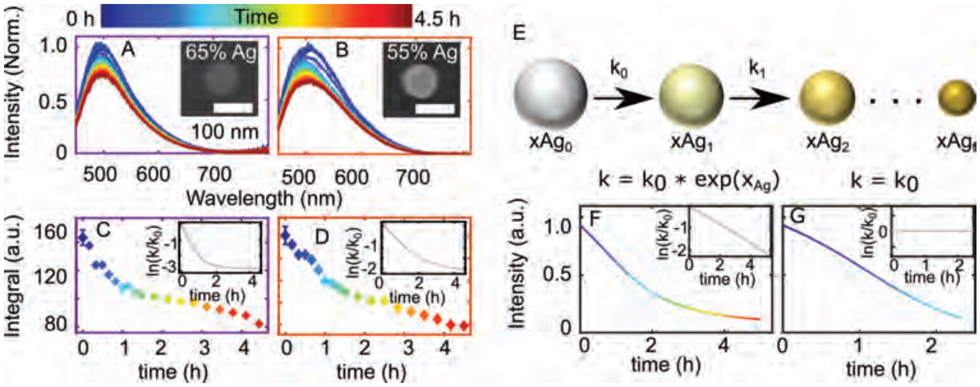

Figure 1: (A, B) Spectra of single Au–Ag nanoalloys during leaching. Inset: Scanning electron microscopy (SEM) image after leaching. (C, D) Leaching profiles over time. Insets: corresponding rate constants. (E) Proposed leaching model. (F, G) Mie theory simulated leaching profiles for the proposed leaching model and a simple shrinking particle model, respectively. Insets: corresponding rate constants. Adapted from Professor Christy Landes.

RESULT

Gold (Au)–silver (Ag) alloy nanoparticles with different amounts of Ag were synthesized using laser ablation. Silver leaching in individual nanoalloys in weakly acidic (0.25 M) nitric acid was monitored by following the changes in plasmon resonance energy as they scatter incident light (Figures 1A and 1B). Spectral changes as leaching occurred were correlated to Ag percentage in each nanoalloy using energy-dispersive X-ray spectroscopy (EDX) of the metal nanoparticles. Particles that initially contained 90% Ag showed no more scattering intensity after 1 h, while pure Ag particles disappeared within minutes, indicating the addition of Au slows down silver leaching. A kinetic model was developed that described an initially fast change in intensity, followed by slower intensity decrease (Figures 1C and 1D). An effective leaching rate was calculated by taking the derivative of the leaching profiles at each point. This analysis revealed two leaching stages: an initial stage where the leaching rate decreases exponentially and depends on the Ag mole fraction, and a second stage where almost no change in the leaching rate happens consistent with a shrinking particle model (Figure 1E). The knowledge of leaching kinetics allows precise nanoparticle tuning, through controlled leaching, to change plasmon resonance energy and electrochemical behavior.

WAY AHEAD

Theoretical leaching profiles for Ag-rich particles and Au-rich particles were constructed with Mie theory, which agreed well with the experimental leaching profiles for the first 2.5 h (Figure 1F). The second leaching stage was not reproduced by the model. Once the Au–Ag alloys contained less than 65% Ag, the gold was able to form continuous unreactive domains. Further leaching thus required the slow diffusion of Ag atoms through the Au layer. When the leaching experiment was repeated in stronger (1.7 M) nitric acid, it was observed that most particles were able to completely release all their Ag under these more acidic conditions. However, about a quarter of all alloys did not leach more than 50% Ag and appeared stable for the duration of the experiment, indicating a strong inter-particle dependence that is hypothesized to be due to an as-yet uncontrolled passivating Au layer. Further research is needed to understand the differences between particles that govern the removal of Ag from particles with lower initial Ag concentration. Ensemble analyses would be incapable of teasing out such heterogeneities such as the above-mentioned super-stable alloys as well as the presence of aggregates with different kinetics. This research seeks to further explore the underlying reasons for the enhanced stability observed for some of the alloy nanoparticles in order to design improved nanoelectrodes.

ARL Competencies:

Energy Sciences

Results

- Collaboration between academic researchers at Rice University and the University of Duisburg-Essen (Germany) suggested that alloy nanoparticles produced by laser ablation provide a facile, up-scalable method for delayed ion release or controlled particle shape/size change.
- Single-particle studies revealed details about nanoalloy reshaping during silver leaching that would not be possible in ensemble experiments.

Anticipated Impact

Mechanistic knowledge and control of nanoalloy leaching kinetics could enable future leap-ahead technologies such as lightweight energy sources and detection of small changes at device interfaces.

This success was made possible by:

Dr. Robert Mantz, Chemical Sciences Branch

Dr. James Parker, Chemical Sciences Branch

Citations:

Wang, Y., *et al. ACS Photonics* **6**, 2295-2302 (2019a).

Wang, Y. *et al. Faraday Discussions* **214**, 325–339 (2019b).

SUCCESS STORY

Hot Electron Injection in Photocatalytic Plasmon-Resonant Nanostructures

ARO funding enabled the observation of new spectroscopic signatures associated with plasmon-resonant hot electrons (in addition to the bulk interband transitions) in metal grating structures on ultra-fast timescales. By comparing these structures in air and in solution, this effort achieved the first spectroscopic evidence that hot electrons are injected into liquid electrolytes using this technique, thereby providing a potential route for a more rapid and economical synthesis of essential compounds for use in fuel cells or batteries.

CHALLENGE

While hot electrons are able to drive difficult chemical reactions, the main challenge associated with hot electrons is that they are short-lived (~2 ps, i.e., 10^{-12} s). The ultra-fast spectroscopic techniques used by Professor Stephen Cronin (University of Southern California [USC]) open up a new way for the exploration of high energy barrier chemical reactions (such as ammonia formation from nitrogen [N_2] or carbon dioxide [CO_2] reduction to hydrocarbons).

ACTION

Dr. Mantz has kept ARO at the forefront of this emerging and promising field. He and Dr. Parker envisioned and sponsored a workshop at Rice University in 2013 to identify key research thrusts. Since then, he has catalyzed ground-breaking work in this area. His support of plasmon-resonant catalysis and electrochemistry led to the support of research that began in 2019 studying "hot electrons," which are capable of driving reactions that extend far beyond that of standard equilibrium chemistry.

RESULT

Professor Cronin and his research team at USC have developed a set of plasmon-resonant nanostructure gratings that distinguish plasmon-resonant excitation from conventional bulk absorption in metals (such as Au, Ag, and copper) simply by rotating the polarization of the incident light and keeping all other aspects of the measurement constant (Figure 2). Ultra-fast transient absorption spectroscopy (TAS) shows the emergence of a new spectroscopic feature associated with plasmon-resonant hot electrons (in addition to the bulk interband transitions) in an Au grating. A spectral blueshift of this hot electron feature is seen in air, while a redshift is seen in solution (Figure 3). This is the first spectroscopic evidence that hot electrons are being injected into the liquid electrolyte using this technique.

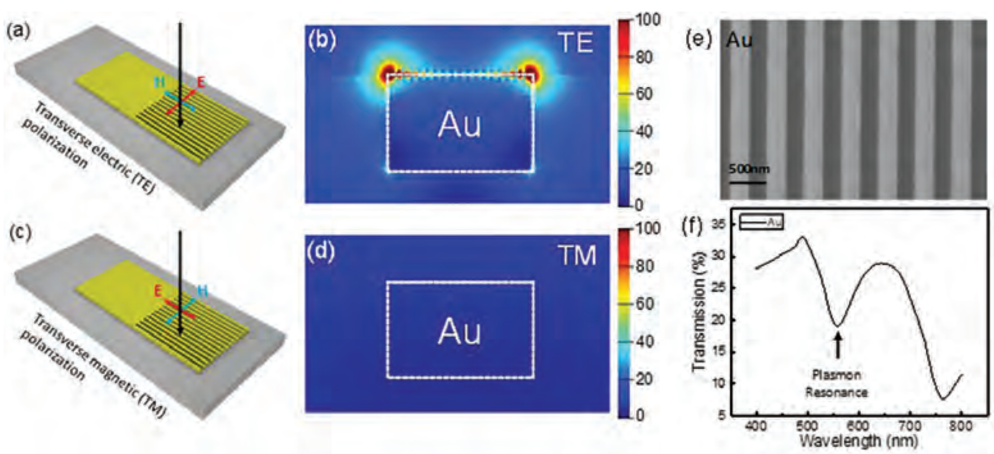

Figure 2: Schematic diagrams of plasmonic metal gratings irradiated with (A) transverse electric (TE) and (C) transverse magnetic (TM) polarized light. Cross-sectional distribution of the electric-field intensity (E^2) of this grating when irradiated with (B) resonant (i.e., TE) and (D) non-resonant (i.e., TM) polarized light. (E) SEM image and (F) ultraviolet-visible transmission spectrum of an Au grating with a 500-nm period. Adapted from Wang et al. (2019a).

WAY AHEAD

The research team is now poised to utilize this approach to extend the study into the liquid domain to explore the energetics of charge transfer using single-electron redox reporters (i.e., molecules whose absorption spectra change when they gain one electron). They will also deposit ultra-thin layers of catalyst materials (e.g., palladium, ruthenium) as metal bilayers to serve as catalytically active, strongly plasmonic nanostructures.

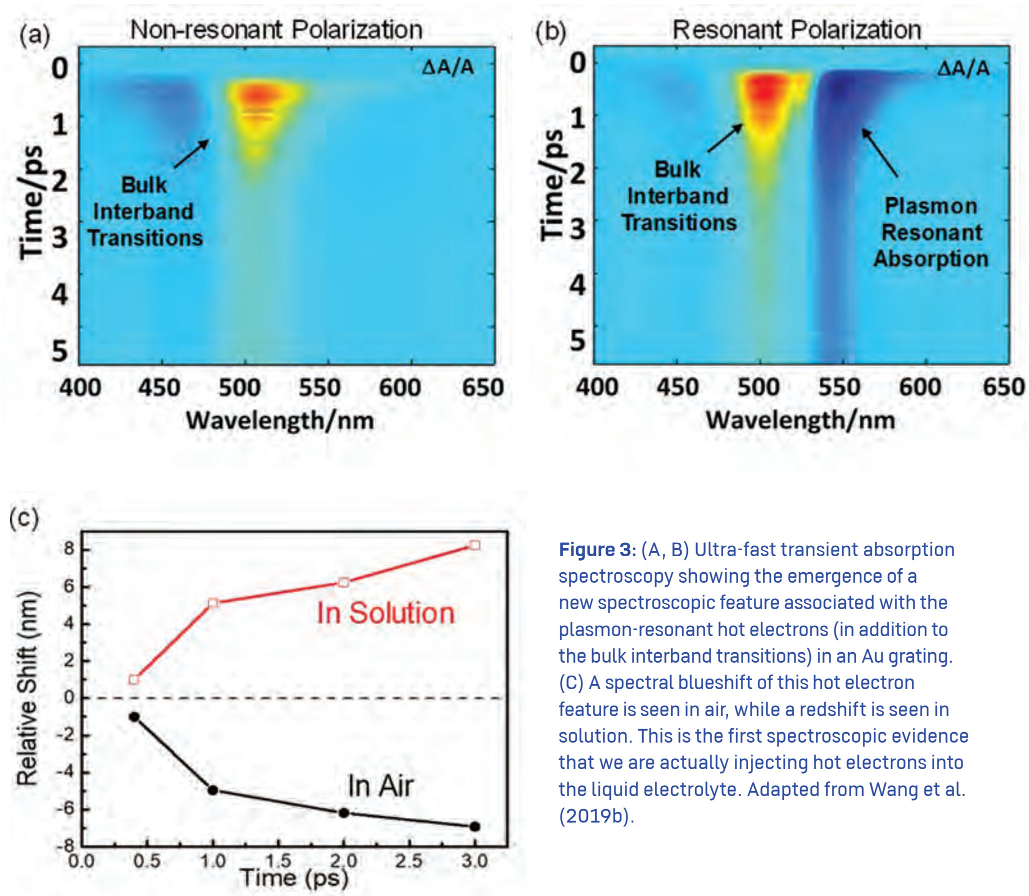

Figure 3: (A, B) Ultra-fast transient absorption spectroscopy showing the emergence of a new spectroscopic feature associated with the plasmon-resonant hot electrons (in addition to the bulk interband transitions) in an Au grating. (C) A spectral blueshift of this hot electron feature is seen in air, while a redshift is seen in solution. This is the first spectroscopic evidence that we are actually injecting hot electrons into the liquid electrolyte. Adapted from Wang et al. (2019b).

ARL Competencies:

Energy Sciences

Results

- ARL and USC co-published a paper in *ACS Omega*.
- Co-hosted an ARL intern through the DoD Historically Black Colleges and Universities/Minority-Serving Institutions (HBCUs/MIs) Internship Program.

Anticipated Impact

Electrochemistry using hot electrons is expected to enable a new way to facilitate high energy barrier chemical reactions, such as ammonia formation from N_2, or CO_2 reduction to hydrocarbons under moderate conditions.

ENVIRONMENTAL CHEMISTRY PROGRAM

Program Manager
Dr. Elizabeth King-Doonan

Dr. King-Doonan completed her undergraduate studies at Boston University, receiving her B.S. in Marine Science in 2012. She trained as a biogeochemist at Oregon State University, receiving her Ph.D. in Earth, Ocean, and Atmospheric Sciences in 2017.

She came to ARO in 2019 as the Program Manager for Environmental Chemistry.

Current Scientific Objectives

1 | Achieve understanding of the structure and reactivity of chemicals in multiphase environments, where reactions and transport processes occur between the solid, liquid, and gaseous phases that, if successful, will mitigate the impact of attacks or disasters by enabling accurate assessment of chemical transport, and thus rapid response by future Army forces.

2 | Develop cutting-edge analytical and experimental approaches to discern compounds of interest in complex environments that, if successful, will enable new capabilities for the detection and source partitioning of threat agents and contaminants.

3 | Advance computational efforts to predict chemical fate, transport, and transformation over a wide range of temporal and spatial timescales that, if successful, will close critical knowledge gaps that limit relating nanoscale chemical reactions to macroscale environmental dynamics.

SUCCESS STORY

Identifying Transport Mechanisms of Volatile Organic Compounds Expected to Improve Protection from Industrial or Wartime Chemical Release Events

This ARO initiative developed experimental methods to accurately measure how volatile organic compounds (VOCs), a ubiquitous class of anthropogenic contaminants, partition between soils, water, and airborne particles. These advancements will enable scientists to accurately detect and predict the fate and transport of toxic compounds, ultimately mitigating civilian and non-civilian exposure following chemical release events.

CHALLENGE

Implementing rapid response strategies and predicting the human health impacts from an accidental or nefarious chemical release event requires an understanding of how contaminants will be transported through various components of the environment, predominately between soils, water, and airborne particulates. VOCs are a class of chemicals that can be released into the environment as a chemical weapon or through the use and disposal of pesticides, fuels, and solvents. In fact, approximately 50-90 million tons of VOCs are released into soils worldwide on an annual basis, making VOCs the most prevalent yet poorly constrained contaminants in the environment (Breus and Mishchenko, 2006).

The challenge with mitigating the effects of VOCs mobilized in the environment is related to the ability to predict how VOCs will distribute across the solid, liquid, and gaseous phases under dynamic environmental conditions. Calculating the distribution of a chemical across multiple media, also known as the partition coefficient, is critical for predicting transport and exposure. While partition coefficients are relatively well characterized at equilibrium, traditional experiments have often overlooked the effect of temperature, humidity, solar radiation, and carbon content. Further, the partition coefficients for many VOCs are extrapolated from studies that focus on only a few semi-volatile organic compounds. Recent studies have shown that partition coefficients for some VOCs are tightly coupled to particle surface chemistry, which, in turn, is a function of a myriad of environmental conditions. Thus, a complete understanding of the fate of VOCs requires a thorough investigation of partition coefficients under realistic conditions, where the synergistic effect of the environment can be fully realized.

This success was made possible by:

Dr. Elizabeth King-Doonan, Chemical Sciences Branch

Dr. James Parker, Chemical Sciences Branch

Citations:

Breus, I. P. & Mishchenko, A. A. *Eurasian Soil Science* **39**, 1271–1283 (2006).

Ahn, J., Rao, G., Mamum, M. & Vejerano, E. *Environ. Chem.* **17**, 545–557 (2020).

ACTION

In 2015, recognizing advances in aerosol chemistry, particularly in the development of environmental chambers capable of mimicking the natural environment, Dr. James Parker (former Environmental Chemistry Program Manager) established a new thrust area focused on the fate and transport of chemical species. The development of this thrust area led to discussions with Dr. Linsey Marr at the Virginia Polytechnic Institute and State University advancing the hypothesis that the partitioning of VOCs between soils, water, and airborne particles would be significantly affected by relative humidity, temperature, and the surface chemistry of soils and airborne particles. The challenge of this research would be to elucidate the effect of each environmental parameter on VOC partitioning, especially under dynamic conditions where multiple variables would be in flux at once. The proposed effort from Dr. Marr would overcome this challenge by designing and fabricating an environmental chamber where conditions could be adjusted to reflect the natural environment and aerosols could be generated with specific chemistries to reflect airborne particles consistent with accidental and deliberate exposure events.

While the proposed effort had clear environmental relevance, Dr. Parker spoke with researchers at the U.S. Army Corps of Engineers, Engineer Research and Development Center Environmental Laboratory to assess how the research could be targeted to optimize Army impact. Through these engagements, it became clear that deciphering reaction mechanisms in complex, heterogeneous systems is a critical knowledge gap for the Army, and while the experimental chamber would be high risk, this effort would potentially provide the first holistic method to accurately measure the fate and transport of VOCs in non-ideal environments. A Single Investigator effort was initiated in 2016.

RESULT

Dr. Marr's approach to precisely measuring VOC partitioning involved coupling the environmental chamber prototype to a gas chromatograph-mass spectrometer (GC-MS) to analyze trace-level concentrations of VOCs captured in each environmental reservoir. In order to attribute partitioning mechanisms to the appropriate variable, an experimental matrix was developed that considered the effect of relative humidity, temperature, soil mineralogy, and soil organic matter content for a suite of six VOCs ranging in polarity; whereby, non-polar compounds have uniform charge and polar compounds have a charge gradient across the molecule. Results were reported by calculating the partition coefficient—the ratio of the concentration of the VOC of interest in one phase to the concentration in another phase. For example, the soil-to-air partition coefficient (K_{SA}) for benzene would be calculated by measuring the concentration of benzene remaining in soil relative to the amount of benzene collected from an air sample in the same environmental chamber.

Over the course of four years, Dr. Marr and her colleague, Dr. Eric Vejerano, have made significant progress elucidating the effect of dynamic environmental conditions on partition coefficients. Focusing on the soil-to-air partition coefficient (K_{SA}), the research team discovered that the effect of changing environmental conditions was largely a function of VOC polarity. Non-polar, hydrophobic VOCs such as 1,2-dichlorobenzene and toluene were more likely to remain in soil enriched with organic matter rather than clay soils, indicating that these VOCs have enhanced affinity for hydrophobic sites on organic matter. At the same time, as the water content of soils increased (i.e., high relative humidity), the K_{SA} decreased, indicating that when water surrounds organic matter in soil, the interaction between organic matter and the VOC compound is reduced. This change in the soil–air interface causes the VOC compound to partition more favorably into air. As VOC polarity increased, the presence of organic matter within soil did not alter the partitioning between soil and air, indicating that polar VOCs were not interacting as strongly with organic matter. Interestingly, for polar VOCs, there was a large spread in the role of humidity on the magnitude of K_{SA}, which the research team attributed to the unique interactions that occur between air and water. These results represent a significant paradigm shift for VOC partitioning, whereby physiochemical models should be developed separately for polar, weakly polar, and non-polar VOCs. These results were published between 2019 and 2020 in *Chemosphere and Environmental Chemistry*.

In 2020, this research further culminated in a study investigating the release of VOCs from a chemical spill in Texas that occurred during Hurricane Harvey. In 2017, Hurricane Harvey dumped massive amounts of rain across south-eastern Texas, and damage during the storm led to the release of 4.6 million pounds of hazardous chemicals into the environment, including the VOCs benzene and toluene. Using temperature and soil water content records from the days immediately following the chemical spill, the research team was able to calculate the appropriate K_{SA} for the released VOCs. Armed with the appropriate partitioning information, the research team subsequently calculated an upper limit of the mass of VOCs present in the soil and released to the atmosphere for the 20 days following the hurricane (Figure 1). When compared to recorded data, the model predicts lower atmospheric concentrations than what was observed, suggested that that multiple chemical spills likely contributed to the spike in VOC concentrations following Hurricane Harvey. These results not only provide precise information to aid in rapid response, but also a potential method for assigning culpability following an environmental disaster.

ARL Competencies:

Humans in Complex Systems

Military Information Sciences

Results

- Achieved understanding of the sensitivity of chemical partitioning between the solid, liquid, and gaseous phases. These results enable precise modeling of individual VOCs in dynamic environments.
- Generated high-resolution detection and prediction capabilities for VOCs released during a chemical spill resulting from Hurricane Harvey in 2017. Results were published in *Chemosphere*.
- Inspired a new ARO program focus area that leverages capabilities in experimental analyses to advance discoveries in chemical structure and partitioning in multiphase environments.

Anticipated Impact

Enhancing capabilities for predicting how chemicals are transported in soils, water, and air is expected to enable future leap-ahead technologies to prevent, reduce, eliminate, and mitigate the release of threat agents in the environment.

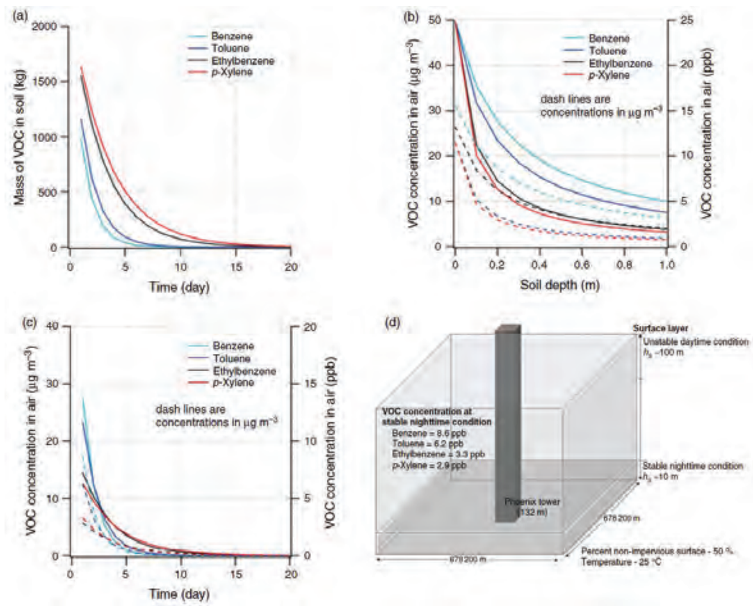

Figure 1: Modeling of VOC fate and transport following Hurricane Harvey: (A) Mass of VOCs remaining in soil, (B) VOCs accumulating in air as a function of soil depth, (C) VOCs accumulated in air under nighttime stable conditions for 20 days following the chemical spill, and (D) the conditions used in the calculations. Adapted from Ahn et al. (2020).

WAY AHEAD

This research represents an important step toward realizing the synergistic effect that dynamic environmental conditions have on the fate and transport of VOCs. Future work will focus on the effect of temperature and relative humidity for synthetic VOCs, including a suite of organophosphates.

Based on the success of this project, Dr. King-Doonan developed a new research thrust area for the Environmental Chemistry Program focused on chemical structure and reactivity in multiphase environments. If the approaches developed in this effort can be applied to a broad swath of chemicals, then this research could have a transformational impact on the Army's ability to detect and predict the fate of harmful chemicals over broad spatiotemporal scales.

This success was made possible by:

Dr. Elizabeth King-Doonan, Chemical Sciences Branch

Dr. Robert Mantz, Chemical Sciences Branch

Citations:

Bland, G. D. & Lowry, G. V. *Anal. Chem.* **92**, 9620–9628 (2020).

SUCCESS STORY

Environmental Forensics for the Detection, Classification, and Transformation of Engineered Nanomaterials

ARO is driving studies that establish methods to discern engineered nanomaterials from natural nanomaterials by coupling environmental chemistry and machine learning techniques. In the long term, these advancements will enable sensitive and rapid identification of the sources and environmental history of engineered nanomaterials based on their unique chemical signature and morphology.

CHALLENGE

Nanomaterials, materials that have at least one dimension of size between 1 and 100 nm, exhibit novel characteristics relative to the same material in bulk form, such as increased strength, conductivity, or reactivity. Nanomaterials can be both naturally occurring (e.g., volcanic ash and soot from wildfires) or engineered (e.g., obscurants, armoring, and self-healing materials). Engineered nanomaterials (ENMs) are often released into the environment, where they can interact with their surroundings and transform based on specific environmental conditions. As global ENM production continues, there are a number of growing environmental concerns regarding their novel characteristics. Specifically, there is evidence that ENMs exhibit increased toxicity relative to their bulk counterparts as they interact with harmful trace metals in the environment. Further, as ENMs degrade and transform in the environment, little is known about the toxicity of their intermediate byproducts.

In order to identify the source and mitigate the effects of ENMs, scientists must be able to identify and track both pristine ENMs and their degraded components. This becomes a challenge in natural environments because both ENMs and natural nanomaterials (NNMs) are made from Earth-abundant elements such as aluminum, iron, silicon, cerium, and titanium. The overlap in chemical composition makes it difficult to find and quantify ENMs present in an environmental medium like soil, which contains high background concentrations of these elements. To fully realize the human health and environmental implications of ENMs, forensic methods are needed to distinguish ENMs from both NNMs and background materials, identify sources, and determine their environmental history.

ACTION

To address the challenges related to locating and sourcing chemicals released into the environment, the most recent former Environmental Chemistry Program Manager, Dr. Robert Mantz, strategically supported research in environmental forensics. These investments targeted experimental methods to discern contaminants from source location to point-of-detection, and developed approaches to predict the degradation of contaminants under various environmental conditions. To advance these efforts beyond individual environments, Dr. Mantz recognized the potential of coupling environmental chemistry with machine learning techniques, and in 2018, he initiated discussions with Dr. Gregory Lowry, a nanomaterials expert at Carnegie Mellon University. Through these conversations, it became clear that discerning ENMs from NNMs in soils was not only a critical knowledge gap in the nanomaterial community, but the ubiquitous nature of ENMs in the environment was also uniquely suited to benefit from the coupling of chemical and machine learning techniques. A Single Investigator effort was initiated on this topic in 2019.

In 2020, Dr. King-Doonan took over as Program Manager for Environmental Chemistry and recognized the important implications that this project had for the environmental forensics community. During a routine update with Dr. Lowry, Dr. King-Doonan's expertise in soil chemistry enabled her to provide valuable insight into the complexities of using Earth-abundant elements as chemical fingerprints. These discussions prompted Dr. Lowry and his research team to investigate the mechanisms driving the transformation of ENMs in soil environments, including the role of mineral–organic particulate interactions and the formation of amorphous mineral precipitates in nanomaterials.

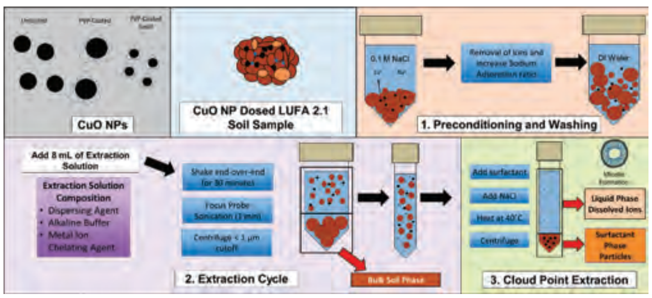

Figure 2: Flow diagram of the nanoparticle extraction protocol. The extraction procedure comprises three steps: (1) preconditioning the soil, (2) extracting colloids/nanoparticles from the soil matrix using sonication and a dispersing agent, and (3) separating the dissolved and nanoparticulate fractions using cloud point extraction. This procedure is the first to extract moderately soluble nanoparticles from soil and experimentally separate them from their dissolved fraction. Figure and caption adapted from Bland and Lowry (2020).

RESULT

To identify ENMs in the environment, the research team first needed to develop a protocol to measure the chemical fingerprint of both ENMs and NNMs. Traditionally, chemical fingerprints are determined by isolating the material of interest from the background material, and measuring the isolated material in bulk on a mass spectrometer where the unique concentrations of certain elements can be used as "fingerprints." In the case of nanomaterials, it would be impossible to physically isolate ENMs from NNMs using traditional methods since they share many physiochemical properties, and Dr. Lowry and his research team were tasked with developing a technique to precisely assign a chemical fingerprint to both materials.

To overcome this challenge, the research team developed the first protocol to effectively extract ENMs and NNMs from soil without simultaneously capturing the dissolved phase of Earth-abundant metals. This three-step extraction procedure was published in 2020 in *Analytical Chemistry* and is summarized in Figure 2. Following this breakthrough, the research team utilized a powerful new analytical tool, the single particle inductively coupled plasma time-of-flight mass spectrometer (spICP-TOF-MS). The spICP-TOF-MS is capable of measuring nearly all elements across the periodic table at ultra-trace levels for an individual particle. These results revealed significant differences in the chemical composition of a single ENM versus a single NNM. The technical achievement of isolating nanoparticulates from a soil matrix and measuring the chemical fingerprint for individual particles paves the way for incorporating machine learning techniques into environmental chemistry. Because the spICP-TOF-MS measures full chemical profiles for individual particles, a single session generates data for thousands of nanoparticles. Future objectives of this effort will focus on developing a machine learning model based on binomial logistic regression to classify ENMs and NNMs from standard and unknown sample sets.

WAY AHEAD

Research leveraging machine learning to overcome challenges in environmental chemistry is still in its infancy. While experimental and theoretical efforts to target known materials and reactions proceed forward at a rapid pace, often these results do not generate ample data to support a fully trained model. Instead, by incorporating machine learning into the method development stage, Dr. Lowry and his research team hope to successfully develop the appropriate methods for ensuring robust scientific determination of ENMs in any type of natural environment. Recognizing this potential, Dr. King-Doonan is pursuing numerous DoD collaborations in conjunction with this work, particularly ARL CISD and DEVCOM SC.

ARL Competencies:

Sciences of Extreme Materials

Results

- Developed pioneering analytical methods to successfully isolate nanomaterials from complex soil matrices. Results published in *Analytical Chemistry*.
- Demonstrated pioneering work to incorporate machine learning techniques to fingerprint and distinguish different sources of nanomaterials using the spICP-TOF-MS.

Anticipated Impact

Pairing environmental chemistry with machine learning is expected to enable future technologies that can provide complete situational awareness in austere environments, where insight into chemical and physical conditions is severely limited.

MOLECULAR STRUCTURE AND DYNAMICS PROGRAM

Program Manager
Dr. James Parker

Dr. Parker completed his undergraduate studies at Marquette University, receiving his B.S. in Chemistry in 1993. He trained as a physical chemist at the University of Mississippi, receiving his Ph.D. in Physical Chemistry in 1999.

He came to ARO in 2009 as the Program Manager for what was then called the Physical and Theoretical Chemistry Program.

Current Scientific Objectives

1 | Achieve control for state-to-state chemical reactions, quantum state preparation, and intermolecular interactions that, if successful, will enable future technologies in keyed detonation of explosives, sensitive and selective chemical threat detection at range, synthetic routes to new energetic materials, and support applications in quantum computing.

2 | Model and explain novel dynamics phenomena, including reaction mechanisms and electron-transfer rates that, if successful, will enable a deep understanding of chemical kinetics, thermochemistry, and catalysis. This information will help to close the gap between how chemical structure and physical properties relate.

This success was made possible by:

Dr. James Parker, Chemical Sciences Branch

Dr. Michael Gerhold, Electronics Branch

Ms. Nicole Fox, Technology Integration and Outreach Branch

SUCCESS STORY

Oxygen Purification via Nanomembrane Separation

A Small Business Technology Transfer (STTR) project was awarded to Global Research and Development Inc. (Global) of Columbus, Ohio, for the development of a portable, on-demand technology to separate oxygen from air for medical applications. The project far exceeded expectations and the company is now positioned to transition the first lightweight, portable, plug-in or battery-operated oxygen purification technology to the commercial market.

CHALLENGE

Pure oxygen is required for medical treatment of patients suffering from a number of acute and chronic health conditions, including, in severe cases, complications from COVID-19. For the Army, a source of medical-grade oxygen is needed in remote field sites to care for wounded Soldiers. There are significant logistical issues in transporting high-pressure oxygen gas cylinders to remote areas. Current Army practice utilizes the technique of pressure swing adsorption (PSA) for production of purified oxygen from ambient air by selective adsorption of nitrogen. However, the equipment is heavy, making it difficult to transport; produces oxygen only at 85–93% pure; and requires significant maintenance. An alternative with significant advantages over PSA and compressed cylinders was sought, including a reliable source of at least 99% pure oxygen.

Since oxygen is used as a standard treatment in hospitals for those suffering from severe symptoms of COVID-19, the task of finishing this project and commercializing it is now even more important, both for civilian and military requirements.

ACTION

In collaboration with Dr. Michael Gerhold, the ARO Optoelectronics Program Manager, Dr. Parker formulated and submitted a topic to overcome these challenges to the Defense Health Agency's (DHA) annual STTR call. The idea centered on the development of a new process for supplying medical-grade oxygen without the use of compressed cylinders or PSA technology. The topic was selected by DHA and published in the Broad Agency Announcement (BAA). Following a successful Phase I STTR, Dr. Parker met with the company president and the principal investigator to better understand the research challenges. Dr. Parker also met with scientific staff at the U.S. Army Medical Research and Development Command (USAMRDC) at Fort Detrick, Maryland, to better understand military requirements for medical oxygen. Serving as a conduit of knowledge, Dr. Parker facilitated information flow between the Army and Global, so that a product meeting DoD requirements could be transitioned. This effort would not have been possible without the assistance of Ms. Nicole Fox, the Program Specialist for the ARO Small Business Innovation Research (SBIR) and STTR Programs, who served as the administrative contracting officer's representative (COR) for this project.

RESULT

Global proposed an alternative idea for oxygen separation from air using a nanoscale thin semi-permeable membrane, which uses a combination of heat and applied electric potential to drive the separation process. Oxygen molecules at the outer surface of the membrane accept two electrons in a reduction process and are separated into atomic oxygen monoanions in the nanomembrane. They flow down their concentration gradient and are oxidatively coupled at the opposite surface from which they are emitted as oxygen molecules. Nitrogen and other species are not carried across the membrane, thereby generating pure oxygen. The working device can be thought of as an oxygen pump (Figure 1). The process has the potential to generate pure oxygen for medical and other applications.

Global is nearing the end of the Phase II portion of this effort and has demonstrated an ability to generate medically pure oxygen at a minimum of 3-LPM flow rate using modest electrical power consumption. Based on the current state of knowledge, it is expected that the company will produce a prototype in the near future.

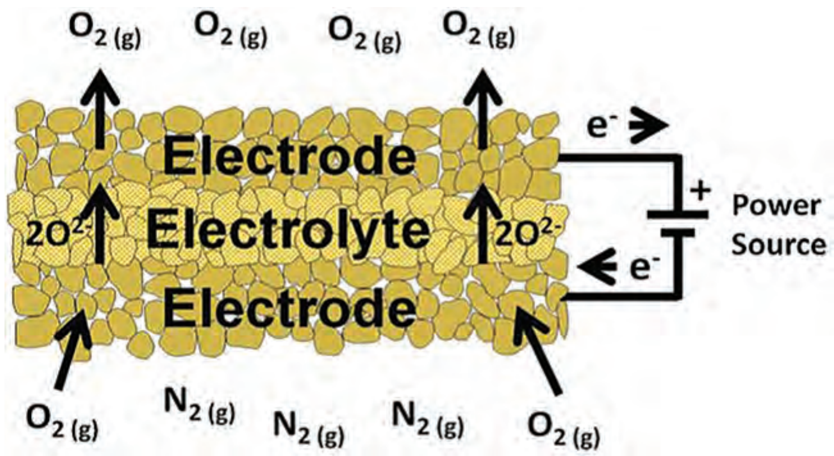

Figure 1: Schematic diagram outlining the operation of an electrochemical cell as an oxygen pump. From Global Research and Development Inc.

WAY AHEAD

During the period of performance of the Phase II project, the COVID-19 pandemic began. Since oxygen is used as a standard treatment in hospitals for those suffering from severe symptoms of COVID-19, the task of finishing this project and commercializing it is now even more important, both for civilian and military requirements. The company is working with private investors on a commercialization plan.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Results

- Developed a technology capable of treating medical patients with an on-demand supply of oxygen nearly anywhere in the world via a portable oxygen generator.

Anticipated Impact

Development of an oxygen purification technology using an electrochemical pump will contribute to saving the lives of Soldiers wounded on the battlefield, especially in locations where logistical problems present challenges to moving heavy equipment.

This success was made possible by:

Dr. James Parker, Chemical Sciences Branch

Dr. Henry Everitt, DEVCOM AvMC

Dr. Jeremy Rice, DEVCOM AvMC

Citations:

Farley III, C. *et al. Proc. SPIE 11498, Photonic Fiber and Crystal Devices: Advances in Materials and Innovations in Device Applications XIV* 114980A (2020).

Roop, L. "Alabama Researchers Find New Ways to Test Aging Army Missiles." *Huntsville Real-Time News.* (2020).

SUCCESS STORY

New Raman Spectroscopic Method to Determine the Reliability of Solid Rocket Propellants in Real Time

Beginning in 2018, Dr. Parker and the DEVCOM AvMC Senior Technologist, Dr. Henry Everitt, determined that the Army would benefit from targeted studies to measure the reliability of solid rocket propellants in aging Army weapons systems. The two agreed that a joint project between Army and academic scientists was needed, and a plan was put in motion to establish a cooperative agreement between Alabama A&M University and the Army.

CHALLENGE

Weapons systems using missile or rocket technology must be reliable over many years of storage in various environments. Over time, the chemical properties of missile propellants can change or degrade, and even result in the missiles becoming unusable. This problem is an ongoing concern for the Army. The usefulness of missile propellants is currently evaluated by being either detonated or decomposed at routine timeframes after many years of storage. Missile propellant samples are extracted from aged missiles and evaluated using multiple chemical analytical methods. These methods are costly and result in the missile being unusable after analysis.

The development of a nondestructive testing method has raised interest in the past decade. Various types of sensors have been considered to assess the aging and usefulness of nitrate ester-based propellants, including those containing nitroglycerin, nitrocellulose, and butanetriol trinitrate. Stabilizers are used in propellants to prolong the usable lifetime of the missile by absorbing free radicals. Stabilizers may include n-methyl-4-nitroaniline (MNA), 2-nitrodiphenylamine (2-NDPA), or diphenylamine (DPA). The stabilizers are gradually depleted over time due to reactions with radicals from various nitrogen oxides (NO_x). The technical challenge is to develop a noninvasive chemical monitoring method. It was decided that the best approach would be to monitor the stabilizer mass fraction over time using various types of spectroscopic sensors.

ACTION

After extensive conversations with Dr. Everitt, it was agreed that a research program involving DEVCOM AvMC scientists and engineers engaging in collaborative research with academic experts in stand-off Raman spectroscopy would be able to meet the challenge of developing a noninvasive, real-time diagnostic test to determine the safety and reliability of solid rocket engines. As the facilitator of the program, Dr. Parker invited a proposal from Dr. Paul Ruffin of Alabama A&M University. Once the proposal was technically reviewed by Army scientists and engineers, it was selected for funding as a cooperative agreement between DEVCOM AvMC and ARO. Drs. Parker and Everitt elected to fund this effort as a cooperative agreement because this award type allows Army scientists to contribute their time and facilities to support the effort.

Figure 2: Raman system probe and propellant sample. Courtesy of Dr. Paul Ruffin.

In February 2020, Dr. Parker conducted a site visit to Alabama A&M University in Huntsville, Alabama. He toured the Physics and Chemistry Department and had briefings from Dr. Ruffin, his research team, and other colleagues in

Figure 3: Live propellant samples. Adapted from Farley III et al. (2020).

the department. This provided Dr. Parker with the opportunity to provide extensive technical feedback to the team. Following the site visit at Alabama A&M, Dr. Parker also toured the DEVCOM AvMC chemistry facilities, where staff analytical chemists gave a detailed briefing of techniques used to monitor the health of missile propellants.

> **"We found optical Raman spectroscopy can look at a missile's propellant to determine whether the missile is still good. The Raman probe can be inserted in the motor, and it shows us whether the propellant in the rocket motor is still useful."**
>
> – Dr. Ruffin, Alabama A&M University senior researcher and adjunct professor (Roop, 2020)

RESULT

This project has been quite successful in developing a spectroscopic method based on Raman scattering, which utilizes a portable Raman spectrometer coupled to the sample via fiber optics. Investigators have chosen to follow the concentration of the stabilizer compound MNA as an indicator of propellant health. Figure 2 shows a Raman spectrometer instrument used in the research. Figure 3 shows some live propellant samples taken from missiles.

WAY AHEAD

A strong collaboration now exists between Dr. Ruffin of Alabama A&M University and Dr. Jeremy Rice of DEVCOM AvMC. This collaboration will ensure fundamental discoveries made possible through ARO will transition throughout DEVCOM for future Army capabilities such as the real-time monitoring of the safety and reliability of rocket and missile weapons systems.

ARL Competencies:

Sciences of Extreme Materials

Results

- Developed a nondestructive method to determine the safety and reliability of solid rocket engines.

Anticipated Impact

This work is expected to enable future leap-ahead technologies such as real-time monitoring of the safety and reliability of rocket and missile weapons systems.

POLYMER CHEMISTRY PROGRAM

Program Manager
Dr. Dawanne Poree
Chief (Acting), Materials Science Branch

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010.

She came to ARO in 2011 as a Systems Engineering and Technical Assistance (SETA) Contractor to support the Polymer Chemistry Program and was hired as the Program Manager in 2014. In addition, Dr. Poree served as the Program Manager (Acting) for Reactive Chemical Systems from 2014-2020.

Current Scientific Objectives

1| Develop new approaches for synthesizing polymers with precisely defined microstructure and composition that, if successful, will enable a deeper understanding of how molecular structure impacts the overall polymer material properties and facilitate the design of polymers with properties of choice.

2| Devise strategies to control polymer assembly and responsive behavior at the molecular level, that, if successful, will render complex materials with programmed and precisely defined functions.

This success was made possible by:

Dr. Dawanne Poree,
Chemical Sciences Branch

Dr. Stephanie McElhinny,
Life Sciences Branch

Citations:

Lee, J., Schwarz, K. J., Kim, D. S., Moore, J. S. & Jewett, M. C. *Nat Commun* **11**, 4304 (2020).

Gerage, A. "Expanding the Palette of Monomers for Ribosome-Mediated Polymerization," *Northwestern.* (2020).

SUCCESS STORY
Toward Sequence-Defined Synthetic Polymers via Engineered Translation Machinery

Using synthetic biology, this ARO initiative is harnessing a cellular macromolecular machine called the ribosome to enable the synthesis of non-natural compounds that may provide a cell-free platform to produce new functional materials and therapeutics.

CHALLENGE

Synthetic biology aims to program biological systems to carry out useful functions, and as a field, has made meaningful progress toward biomanufacturing of medicines, sustainable chemicals, and advanced fuels, as well as cellular diagnostics and therapies. At the core of these advances is the ability to control and tune the processes of transcription and translation, potentially offering access to non-natural materials that cannot be made by any other means. As an example, the translation apparatus is the biological cell's factory for protein synthesis. The ribosome, the molecular machine that polymerizes α-amino acids into proteins, is the catalytic workhorse of the translation apparatus. With protein synthesis rates of up to 20 amino acids per second at an accuracy of 99.99%, the extraordinary catalytic capacity of the translation machinery has attracted extensive efforts to repurpose it for novel functions. While most efforts have focused on the site-specific incorporation of unnatural α-amino acids into proteins by the natural translation apparatus, the chemical space that might be accessible upon engineering the ribosome is virtually unexplored.

ACTION

In 2015, recognizing emerging advances in synthetic biology and particularly the development of in vitro systems capable of modifying biological translation machinery, Dr. Poree and Dr. Stephanie McElhinny (Program Manager, Biochemistry) conceived of a Multidisciplinary University Research Initiative (MURI) topic focused on re-engineering the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner. Sequence-defined polymers (SDPs) are linear macromolecules whose chemical and physical properties can be programmed with atomic-scale resolution. It has been impossible, so far, to produce finely tailored non-natural SDPs (i.e., materials of defined atomic sequence, exact monodisperse length, and programmed stereochemistry), yet the development of synthetic routes toward these molecules promises technological breakthroughs in advanced functional materials, nanotechnology, electronics, and beyond. To achieve this ambitious goal, Drs. Poree and McElhinny brought together a team of researchers, with expertise in synthetic biology, evolutionary biology, synthetic chemistry, and chemical engineering, to develop novel biosynthetic platforms that enable the generation and evaluation of modified ribosomes and other translation factors in a non-cellular, in vitro setting. This dramatically expands the ribosome design space accessible to the team, as ribosomes are essential for cell viability and only limited ribosome mutations are possible in cells. With these modified ribosomes in-hand, the team would then seek to explore their ability to enable non-traditional polycondensation reactions (beyond amide and ester bonds) to render novel, non-natural SDPs.

RESULT

This fiscal year, significant advancements were made toward achieving the overarching goals of this program. More specifically, the research team, led by Professor Michael Jewett of Northwestern University, developed a system to rapidly create and evolve ribosomes in a test tube, alleviating cell viability constraints (Lee et al., 2020). This novel system, termed ribosome synthesis and evolution (RISE), represents a critical step toward designing and modifying the ribosome to work with non-natural substrates. The RISE system allows for making millions to billions of mutant ribosomes within hours, and even more notably, can allow for selecting ribosomes with functions of choice. Separately, the team also sought to gain an understanding of the plasticity of the ribosome. In a first-of-its-kind study to comprehensively dissect the ribosome active site, the research team characterized and mapped the nucleotides of the ribosome active site and explored which ones could be altered without impacting ribosomal activity (Figure 1). To conduct these studies, the researchers employed a previously developed integrated synthesis, assembly, and translation (iSAT) platform that allows for interrogation and manipulation of the ribosome in a manner that mimics the natural cell-like process, but in an in vitro environment. Using iSAT, the team constructed and then tested every possible single nucleotide mutation, 180 in total, in the active site to determine which nucleotides could be changed without "breaking" the ribosome. Surprisingly, it was found that >85% of the active site nucleotides could be altered and still retain activity, offering transformational insights into how the ribosome can be re-engineered to create new materials beyond what is currently possible.

Figure 1: Mutational mapping of ribosome active site. Adapted from Lee et al. (2020).

Concurrently, the research team also sought to establish the design rules that guide the incorporation of non-natural monomers into the engineered ribosomes. Critical to this effort is the ability to link the monomers to transfer RNAs (tRNAs), which are the molecules that deliver the monomers to the ribosome for protein (polymer) synthesis. To achieve monomer–tRNA coupling, the team employed a recently developed RNA enzyme called flexizyme that allows for easier and more flexible monomer attachment, and sought to establish the design rules for flexizyme-mediated coupling. To develop the design rules, the researchers synthesized 37 monomers based on 4 chemically diverse scaffolds (phenylalanine, benzoic acid, heteroaromatic, and aliphatic monomers) that are currently inaccessible to natural ribosomally

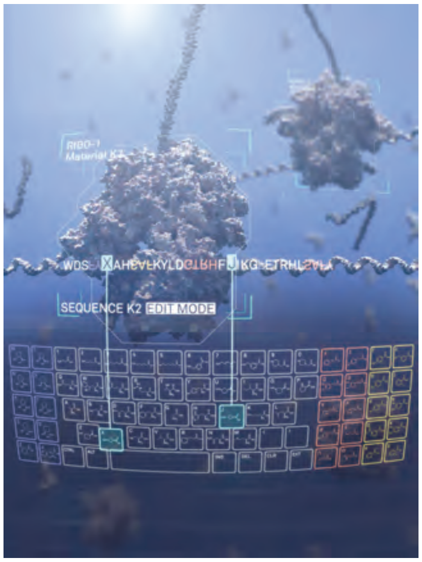

Figure 2: Selection and incorporation of long-chain carbon and cyclic monomers for ribosome-mediate polymerization. Adapted from Gerage (2020).

ARL Competencies:

Biological and Biotechnology Sciences

Results

- Established the design rules to guide how ribosomes can incorporate non-natural monomers.
- Developed the RISE system, which can rapidly create hundreds of engineered ribosomes in vitro and screen/select a specific ribosome to perform a specific function.
- Using these engineered ribosomes, demonstrated the ability to incorporate designer backbone-extended and cyclic amino acids into peptides.

Anticipated Impact

If successful, this work will, in essence, bring synthetic materials into the realm of biological functions and potentially render advanced, high-performance materials capable of catalysis, molecular encoding and data storage, nanoelectronic properties, and self-healing, among many other functions.

synthesized peptides, and explored how their varying electronic and steric factors impacted coupling and subsequent ribosome-directed polymerization. The studies revealed that electron-deficient monomers have more favorable coupling compared to those that are electron-rich, and certain bulky substituents incompatible with coupling were also identified. To validate these design rules, the research team predictably guided the search for new monomers compatible with the flexizyme approach and successfully identified six additional monomers that could be coupled to tRNA and incorporated into peptides via ribosomal polymerization. Guided by these design rules, the research team then demonstrated that a wide variety of backbone-extended (long-chained carbon structures) and cyclic monomers could undergo site-specific incorporation into peptides (Figure 2), thus expanding the scope of ribosome-mediated polymerization and setting the stage for new classes of materials and therapeutics.

WAY AHEAD

The ability to access broader classes of non-natural monomers for ribosome-mediated polymerization opens the door to tackling the "holy grail" of polymer science, which is the synthesis of polymers in a sequence-defined manner. This, in turn, could lead to the creation of materials and therapeutics with very precise and predefined properties and activities. Future research efforts will continue to focus on expanding the monomer chemistry accessible to ribosome-mediated polymerization and will also begin exploring co-monomer polymerization. Collaborative efforts among ARO and the ARL Transformational Synthetic Biology for Military Environments (TRANFORME) Essential Research Program will be sought to transition key knowledge products toward the development of new synthetic biology techniques to enable novel materials and processes for future operating environments.

This success was made possible by:

Dr. Dawanne Poree,
Chemical Sciences Branch

Citations:

Estabrook, D. A. & Sletten, E. M. *ACS Cent. Sci.* **6**, 1482–1484 (2020).

Ahn, D., Stevens, L. M., Zhou, K. & Page, Z. A. *ACS Cent. Sci.* **6**, 1555–1563 (2020).

SUCCESS STORY

Rapid, High-Resolution 3D Printing Using Visible Light

This ARO initiative resulted in a rapid and precise 3D printing method that uses visible light, opening the door to next-generation designer materials manufacturing. Whereas current 3D printing methods rely on ultraviolet (UV) light to photocure the polymer, the new method uses visible light from light-emitting diodes (LEDs) that is compatible with a wider array of materials and requires the same light source as found on a mobile phone. This improved LED-based 3D printing method paves the way for new materials for use in areas such as soft robotics, functional coatings, and prosthetics.

CHALLENGE

There is currently much interest in 3D printing of materials as an "on demand" means of manufacturing useful devices, which promises to revolutionize fields such as machining, medicine, and consumer goods, to name a few. As such, 3D printing may be particularly enabling for DoD applications where manufacturing at the point of use may provide unique capabilities and ease supply chain and logistics issues. Though significant advances in 3D printing have been made, there remain several classes of materials for which additive manufacturing has yet to be realized, due in large part to a lack of curing approaches that are compatible with functional materials.

ACTION

In 2015, recognizing the ubiquitous nature of polymeric materials, Dr. Poree began focusing programmatic resources on novel approaches for integrating functional polymeric materials with additive manufacturing processes. Of particular interest was expanding photocuring approaches beyond the traditional UV light-based curing processes. While UV light is highly advantageous for its rapid curing capabilities, it requires high energy intensity and is limited in its materials scope. Conversely, recent advances in photopolymerizations have demonstrated visible light photochemistries as a lower-energy (and thus more cost-effective), tunable, and also more biocompatible and functional group tolerant alternative, thus offering access to a broader range of materials. Despite these advantageous attributes, visible light photochemistry currently suffers from slow reactions times, high intensity irradiation, and/or high catalyst loading, which precludes its utility in photocuring applications such as 3D printing. To address this challenge, Dr. Poree strategically supported Professor Zachariah Page at the University of Texas at Austin to explore how photocatalyst composition impacts polymerization rates when activated by low-energy wavelengths of light, with the goal of identifying and developing photoredox catalysts that enable rapid and efficient curing using visible light.

RESULT

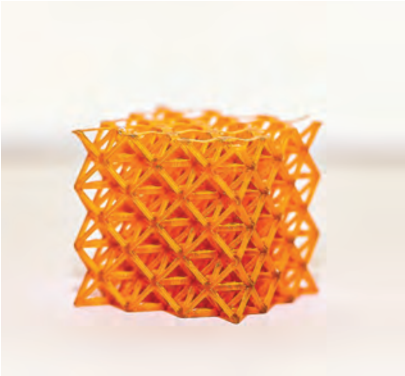

Figure 3: Rapid high-resolution DLP 3D print of a hierarchical octet-truss lattice using a BODIPY-bromine derivative as the photocatalyst and a green LED centered at 530 nm as the light source. Adapted from Ahn et al. (2020).

In FY20, the research team sought to explore boron dipyrromethene (BODIPY) as a potential photocatalyst platform for visible and near-infrared (NIR) polymerizations (Ahn et al., 2020). BODIPY dyes demonstrate a wide range of optoelectronic properties with peak absorption values from 500-900 nm. Additionally, halogenation of BODIPY dyes is known to generate long-lived excited triplet states, which increases photocatalytic efficiency, potentially rendering these compounds as ideal candidates for visible to NIR photocuring. To test this hypothesis, a series of methine- and aza-bridged BODIPY dyes were synthesized and subsequently halogenated to render chlorine, bromine, and iodine derivatives, and then systematically characterized to elucidate key structure–property relationships that facilitate efficient photopolymerization driven by visible to far-red light. For both BODIPY scaffolds, halogenation was shown as a key mechanistic step and thus a generalizable method to achieving rapid photopolymerization reactions, demonstrating 5-8 times higher polymerization rates relative to the non-halogenated derivative. Results further revealed unprecedented polymerization rates (complete conversion within 60 s) using extremely low light intensities and catalyst loadings (<1 mW/cm^2 and ~0.001 mol%, respectively). As these rapid kinetics are ideal for photocuring applications, the team further sought to demonstrate the feasibility of these BODIPY photocatalysts to enable rapid 3D printing with visible light. Figure 3 shows a complex 3D printed structure using the BODIPY catalyst (bromine derivative) at 530 nm. An exposure time of 10 s per layer rendered good resolution and also corresponds to a build rate of 9 mm/h, making it competitive with state-of-the-art commercial digital light processing (DLP) 3D printers that rely on high-energy UV light.

Concurrently, the research team also sought to develop novel photopolymer resins with rapid reaction kinetics upon irradiation with light across the visible spectrum. More specifically, the resin systems comprised a monomer, a photoredox catalyst specific to the desired wavelength of photocuring, electron-deficient and electron-rich co-initiators to enhance photocuring efficiency, and azo dyes to confine curing to only the areas irradiated by light to render improved spatial resolution. Employing four different photoredox catalysts that each absorb at different wavelengths of light and a DLP 3D printer constructed with exchangeable LEDs, the team demonstrated that the developed resins could be rapidly cured using red, green, blue, or violet light (depending on the photocatalyst used) and could also be patterned to build objects in a layer-by-layer fashion (Figure 4). Additionally, by using different monomers (poly[dimethyl acrylamide] and 2-hydroxyethyl acrylate), the mechanical properties of the materials could be tailored from stiff or soft. The resulting printed objects could also achieve feature sizes <100 µm with build speeds up to 45 mm/h, which is close to parity with the state-of-the-art UV-based printing technologies.

Figure 4: Digital image of longhorns 3D printed with different colors of low-energy visible light. From left to right: blue, green, and red light were used to rapidly solidify the resin by activating the corresponding catalysts shown above each print. A quarter is present to the far left for reference, showing the high-resolution capabilities possible with this 3D printing process. Adapted from Ahn et al. (2020).

WAY AHEAD

The next research objective is to utilize the design parameters identified in these studies to extend this photochemistry into the NIR. Collaborative efforts among ARO, ARL WMRD, and DEVCOM SC will be sought and leveraged to transition key knowledge products toward the development of new functional materials for coatings, adhesives, structural elements, wound dressings, and fabrics.

ARL Competencies:

Sciences of Extreme Materials

Results

- Demonstrated halogenated BODIPY derivatives as a viable photocatalyst platform for visible light-based photocuring.
- Developed novel panchromatic photopolymer resins and applied for the first time to realize rapid high-resolution visible-light 3D printing.
- Developed a versatile and general visible light-based printing methodology that rivals state-of-the-art UV-based printing technologies, demonstrating feature sizes <100 µm, build speeds up to 45 mm/h, and mechanical isotropy.

Anticipated Impact

These foundational studies lay the groundwork for further development of visible and NIR photocuring, which has the potential to enable next-generation designer materials manufacturing to include bio- and composite-based 3D printing, which are currently inaccessible with existing UV curing methodologies. Additionally, this work also lays the foundation for wavelength selective photocuring to generate on-demand, multi-material structures with discrete and spatially defined chemical and mechanical properties.

REACTIVE CHEMICAL SYSTEMS PROGRAM

Program Manager (Acting)
Dr. Dawanne Poree
Chief (Acting), Materials Science Branch

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010.

She came to ARO in 2011 as a Systems Engineering and Technical Assistance (SETA) Contractor to support the Polymer Chemistry Program and was hired as the Program Manager in 2014. In addition, Dr. Poree served as the Program Manager (Acting) for Reactive Chemical Systems from 2014-2020.

Current Scientific Objectives

1 | Create chemically and biologically functionalized surfaces with precise control of structure and function that, if successful, are anticipated to lead to novel decontaminants, sensors, and coatings for Soldier protection.

2 | Attain a mechanistic understanding of mass transport, adsorption, and reactivity on surfaces and at interfaces that, if successful, is anticipated to lead to novel materials and catalysts for degrading chemical threats.

3 | Design and synthesize chemical systems that sense and respond to external stimuli that, if successful, are anticipated to lead to intelligent materials for Soldier protection.

This success was made possible by:

Dr. Dawanne Poree,
Chemical Sciences Branch

Dr. John Prater (retired),
Materials Science Branch

Citations:

Meredith, C. H. *et al. Nat. Chem.* **12**, 1136–1142 (2020).

SUCCESS STORY
Chasing Droplets: Predator–Prey Interactions

ARO-funded research in synthetic molecular systems resulted in the demonstration of micelle-mediated oil exchange to drive predator–prey interactions between droplets. This discovery provides a notable advancement in future sense-and-respond systems that will enable new protection capabilities for the future Soldier.

CHALLENGE

Biological systems, such as organisms, are dynamic and adaptive, and can communicate via diverse pathways. While more conventional materials have been pursued to mimic "living" behaviors, it remains a significant challenge to achieve equivalent complexity in artificial systems. Liquids are dynamic and reconfigurable. Mixtures of immiscible liquids, or emulsions, offer a unique opportunity to control chemo-mechanical feedback, signal amplification, and chemically mediated interactions between droplets. To exploit the full potential of fluid materials, a fundamental understanding of the dynamics at liquid interfaces in multiphase fluids needs to be attained.

ACTION

To address one of the program's objectives of designing sense-and-respond systems, ARO Reactive Chemistry Systems Program Manager, Dr. Poree (acting), strategically supported research in synthetic molecular systems. These investments encompassed the synthesis of new responsive systems based on polymer, liquid crystal, and hybrid materials, and the development of state-of-the-art tools and methods to directly visualize dynamic behavior in real time. To achieve the response rates and selectivities required for utility, projects were also identified that focused on approaches to amplify a singular molecular-scale detection event to a macroscopically observable response. Dr. Poree recognized the scientific innovation of emulsions as dynamic materials, and initiated a Young Investigator Project (YIP; now Early Career Program [ECP]) award with Professor Lauren Zarzar at The Pennsylvania State University (Penn State), followed by a Presidential Early Career Award for Scientists and Engineers (PECASE) nomination. In FY19, Professor Zarzar received an Army Early Career Award for Scientists and Engineers (ECASE) award to study adaptive fluid materials (transition to PECASE subject to White House approval).

RESULT

In FY20, the Penn State research team studied pair-wise and multi-body interactions between oil droplets of differing chemistry in aqueous surfactant and found that due to micelle-mediated oil transport, droplets can “chase” each other, simulating natural predator–prey interactions.

Interactions between chemically distinct, microscale oil droplets in micellar surfactant solutions were investigated. In a non-ionic, aqueous surfactant solution, it was observed that 1-bromooctane (BOct, the predator droplet) was attracted to and accelerated toward ethoxynonafluorobutane (EFB, the prey droplet), and EFB moved away in response (Figure 1). Within tens of seconds, EFB was “caught,” resulting in the formation of motile droplet pairs and droplet clusters with speeds up to 20 μm/s and sustained interactions greater than an hour. Control experiments in which either of the oil droplets were replaced with similarly sized polymer particles or droplets of only a single oil type did not result in the same dynamic behavior. It is proposed that the energy driving the motion is primarily from the entropy of mixing due to micelle-mediated oil exchange between the droplets. By varying the droplet and surfactant structures and concentrations, the interactions between the droplets can be regulated. Increasing the surfactant concentration demonstrated stronger chasing interactions. Substituting the original surfactant with a non-ionic, *fluorinated* surfactant reversed the chasing behavior: EFB acted as the predator and BOct became the prey droplet. Other fluorinated oils having partial miscibility with BOct resulted in similar interactions as those observed with EFB; however, the motion subsided when an oil with limited miscibility with BOct, such as perfluorohexane, was used. Studies at higher droplet densities with the same BOct/EFB/surfactant system revealed that chasing pairs interact and assemble into clusters. These multi-body interactions continued to evolve over minutes, suggesting that chemical signaling or communication pathways may exist in complex droplet networks. A manuscript highlighting this research has been accepted in *Nature Chemistry.*

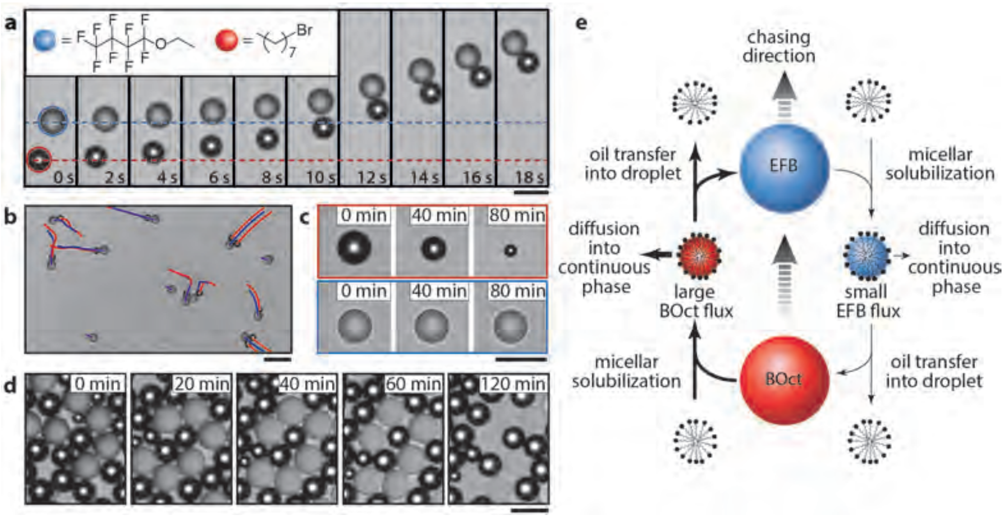

Figure 1: BOct droplets chase EFB droplets in aqueous surfactant. (A) Time-sequence frames of chasing interactions between the BOct predator droplet (red) and EFB prey droplet (blue) in 0.5 wt% Triton X-100 aqueous solution; (B) Trajectories of BOct drops (red lines) EFB drop (blue lines) over 30 s showing linear motion of pairs and multi-droplet clusters; (C) Optical micrographs of the isolated BOct droplet (top) versus the EFB droplet (bottom) in 0.5 wt% Triton over time; (D) When mixing BOct and EFB droplets in aqueous surfactant, the refractive index of EFB increased over time, eventually becoming nearly transparent and swelling in size (100 μm scale); (E) Hypothesized mechanism wherein chasing interactions are associated with micelle-mediated oil exchange, where the flux of BOct is much greater than that of EFB in 0.5 wt% Triton due to BOct’s higher micellar solubilization rate. Adapted from Meredith et al. (2020).

WAY AHEAD

The ability to design synthetic systems with characteristics typically inherent in biological systems will significantly contribute to the advancement of dynamically reconfigurable soft materials. The research has demonstrated a platform to manipulate the predator–prey interactions of a simple oil-in-water model system. With continued support from ARO, Penn State researchers will persist in exploring emergent phenomena in emulsions aimed at developing predictive pathways for designing collective organization and non-equilibrium dynamics. Droplets containing more than one oil, such as Janus droplets, or droplets containing reagents that react over time to create chemical gradients can provide additional tunable control over droplet organization and morphology. Collaborative efforts among ARO, ARL WMRD, the Institute for Collaborative Biotechnologies (ICB), and the Defense Threat Reduction Agency (DTRA) will be sought and leveraged to transition key knowledge products for the advancement of new protection capabilities for the Soldier.

ARL Competencies:

Sciences of Extreme Materials

Results

- Demonstrated biological-like signaling and motion between chemically distinct oil droplets in micellar surfactant solutions resulting in predator–prey-like chasing interactions.
- Established a simple, robust platform to tune the predator–prey interactions of a model system.
- Key manuscript published in *Nature Chemistry*.

Anticipated Impact

The design of dynamically reconfigurable soft materials will enable new protection capabilities for the Soldier such as chemical and biological sensors, dynamic camouflage, remote diagnostics, triggered release, and adaptive optics.

This success was made possible by:

Dr. Dawanne Poree,
Chemical Sciences Branch

Citations:

Lu, Y. *et al*. *Nat. Catalysis* **2**, 149-156 (2019).

SUCCESS STORY

Reactivity Descriptors of Single-Atom Catalysts

ARO initiatives led to the discovery of analogous mechanistic pathways for low-temperature carbon monoxide (CO) oxidation with iridium (Ir) single atoms, which provide new routes for responsive materials for next-generation electronics and catalysts for detecting and inactivating toxic threats.

CHALLENGE

Supported metal nanostructure catalysts are critical for a variety of applications including environmental remediation, energy platforms, and pharmaceutical development. Despite their wide employment, supported metal catalysts typically comprise a mixture of nanoparticles and sub-nanometer clusters, and this heterogeneity can reduce catalytic efficiency, trigger undesired side reactions, and make identification of the active site problematic. Recently, there has been significant interest in single-atom catalysts (SACs), where isolated metal atoms are singly dispersed on supports, maximizing atom utilization efficiency and offering unique electronic properties. While literature has shown individual studies of metal-supported catalysts, there are minimal reports of a systematic study comparing metal identity, metal nuclearity (nanoparticle, sub-nanometer cluster, or single atom) and support, and their impact on both catalytic activity and selectivity.

ACTION

To address one of the program's objectives of understanding reactivity on nanostructured surfaces, ARO Reactive Chemistry Systems Program Manager (acting), Dr. Poree, strategically supported research in supported metal catalysts. These investments encompassed synthetic methods toward nanostructured catalysts with well-defined morphologies and function, as well as novel spectroscopic tools/techniques to characterize the catalyst in its active working state. To advance reactive and selective catalytic materials beyond more traditional bulk materials, Dr. Poree identified SACs as a new focal area and initiated a Single Investigator project with Professor Ayman Karim at Virginia Polytechnic Institute and State University (Virginia Tech) to begin differentiating the mechanisms and catalytic properties of metal atoms and small clusters. The research team uncovered the structure and reaction mechanism responsible for the higher catalytic efficiency for low-temperature oxidation of CO observed with Ir SACs compared to Ir nanoparticle catalysts. Despite initial advances in understanding the properties of SACs, the grand challenge of predicting SAC activity and selectivity, even for simple reactions, still remains.

RESULT

Previous research highlighted in Professor Karim's 2019 *Nature Catalysis* publication demonstrated the first proven mechanism for CO oxidation on supported SACs using Ir/magnesium aluminate ($MgAl_2O_4$). In FY20, Virginia Tech researchers expanded their studies to other structural features such as metal identity and metal support to identify potential trends for predicting the activity of supported SACs.

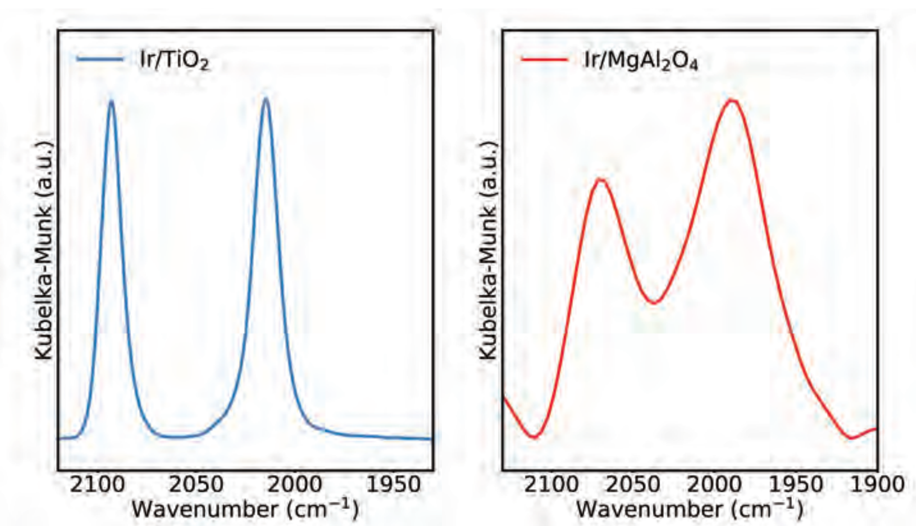

Figure 2: Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) of CO adsorbed on Ir single atoms on TiO_2 (A) and $MgAl_2O_4$ (B) at 35 °C. Image courtesy of Professor Karim.

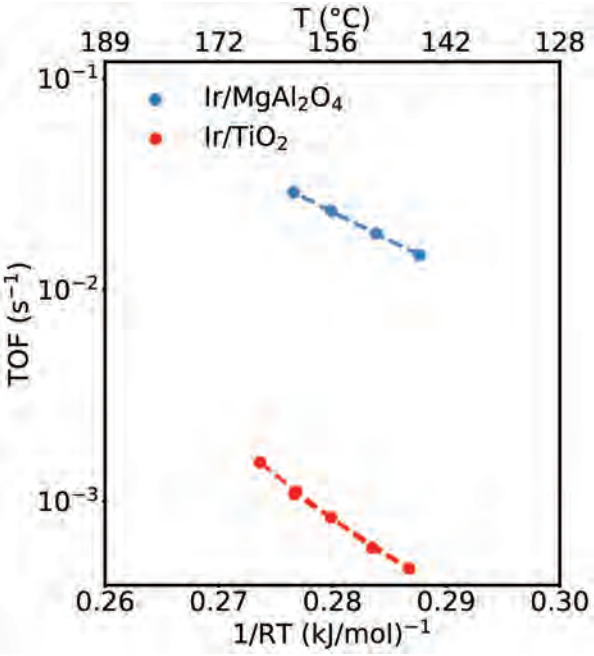

Figure 3: CO oxidation activity of Ir single atoms on TiO_2 (red) and $MgAl_2O_4$ (blue). Image courtesy of Professor Karim.

The effect of adsorbing Ir single atoms on titanium dioxide (TiO_2), a reducible support, was investigated and compared to the results obtained with $MgAl_2O_4$, a non-reducible support. Using a combination of state-of-the-art *in situ* spectroscopic tools and quantum chemical calculations, critical features for CO oxidation were discovered that were analogous to the mechanism identified with the catalyst Ir/$MgAl_2O_4$. Before reaction, the infrared spectra revealed two bands at 2093 and 2014 cm^{-1}, confirming $Ir(CO)_2$ formation (Figure 2), followed by transformation to Ir(CO), the active supported complex during CO oxidation. Upon switching reaction conditions to ^{13}CO and O_2, the most stable intermediate, or catalyst resting state, was identified to be $Ir(^{12}CO)(O)$, confirming that one CO ligand remains attached to the Ir single atom through the entire reaction cycle. Despite the similarities in the reaction pathway, preliminary results from kinetic studies show that Ir single atoms on TiO_2 are much less active than those on $MgAl_2O_4$ (Figure 3). Experiments are ongoing to elucidate the observed activity differences.

WAY AHEAD

Understanding atomic-level mechanistic details of supported SACs will lay the foundation toward designing novel catalysts with superior activity and selectivity for the detection and destruction of toxic industrial chemicals and chemical threats. While research has previously noted differences in mechanism and ultimately activity by varying metal nuclearity, preliminary data suggests that changes to the support in the Ir single-atom system does not alter the reaction pathway but can significantly impact activity. With continued support from ARO (Dr. Poree) and DEVCOM CBC, Virginia Tech researchers will probe the effect of metal-support interactions on CO activity and the reaction mechanism, and identify supported catalyst descriptors toward predicting activity for more complex systems and reactions. Collaborative efforts among ARO, ARL WMRD, DEVCOM CBC, and DTRA will be sought and leveraged to transition key knowledge products to advance new protection capabilities for the Soldier.

ARL Competencies:

Sciences of Extreme Materials

Results

- Results led to ARO collaborations across the DoD, including co-managing three new FY20 cooperative agreements, including a Virginia Tech team (co-principal investigator Professor Karim), with DEVCOM CBC as part of the joint DTRA-CBC program focused on designing small-cluster catalysts.
- Discoveries led to joint ARO-CBC-AFOSR workshop on SACs to be held in FY21 (originally scheduled for FY20 but delayed due to COVID-19).

Anticipated Impact

Single-atom and small-cluster catalysts are expected to enable novel catalytic materials with superior activity and selectivity for the detection and destruction of toxic industrial chemicals and chemical threats; fast, efficient energy conversion; and next-generation electronics.

BIOCHEMISTRY PROGRAM

Program Manager
Dr. Stephanie McElhinny

Dr. McElhinny completed her undergraduate studies at Gannon University, receiving her B.S. in Chemistry in 1999. She trained as a biochemist at the University of North Carolina at Chapel Hill, receiving her Ph.D. in Biochemistry in 2004 and conducted postdoctoral research in biochemistry and yeast genetics at the National Institute of Environmental Health Sciences.

She came to ARO in 2009 as the Program Manager for Biochemistry.

Current Scientific Objectives

1 | Develop approaches to engineer and control mechanisms underlying biomolecular specificity and regulation that, if successful, are anticipated to lead to novel biosensing reagents and responsive materials.

2 | Design self-assembled biomolecular architectures to support functional organization of biological molecules that, if successful, are anticipated to lead to novel power and energy systems and onsite manufacturing capabilities.

3 | Understand sequence-structure-property relationships in biological and biohybrid materials that, if successful, are anticipated to lead to rationally designed materials with tailored properties ranging from therapeutics to adaptive structural materials to protect the Soldier.

This success was made possible by:

Dr. Stephanie McElhinny,
Life Sciences Branch

Citations:

"Army Project Turns to Nature for Help with Self-Healing Material," *DEVCOM ARL Public Affairs.* (2020).

Pena-Francesch, A., Jung, H., Demirel, M. C. & Sitti, M. *Nat. Mater.* **19**, 1230–1235 (2020).

SUCCESS STORY
A Protein-Based Material Capable of Rapid Self-Healing

The ARO Biochemistry Program portfolio identified and supported research focused on unlocking the link between protein sequence and biomaterial properties, which identified a protein sequence that enables self-healing in less than 1 s. This discovery will set the foundation for future protein-based materials that would be ideally suited for systems that require repetitive movement such as soft robots, personal protective equipment, and prosthetics.

CHALLENGE

Soft, flexible polymeric materials are used in a variety of Army-relevant systems, including soft robots and personal protective equipment. While these materials can generally resist blunt damage caused by impact, bending, or compression, they are vulnerable to mechanical damage such as punctures, cuts, and tears due their inherent softness. This limits the lifetime of these materials and the systems in which they are deployed. To extend the useful lifetime of these soft materials, efforts have focused in recent years on self-healing approaches that could repair damage as it occurs. However, current strategies require complex chemical reactions that often utilize toxic materials, require long healing times (often more than 24 h), or require high energy input to trigger the self-healing process. More critically, self-healed materials typically exhibit reduced mechanical strength at the site of healing, rather than recovering the original material properties. In contrast to these soft synthetic polymeric systems, biology demonstrates an ability to self-heal a variety of both hard and soft materials with high efficiency and no loss in material performance post-healing.

ACTION

In 2015, Dr. McElhinny received a white paper from Professor Melik Demirel at The Pennsylvania State University that was focused on squid ring teeth (SRT) protein as a novel biomaterial. Professor Demirel had demonstrated that natural SRT protein variants could be processed into a variety of different material forms, including films, foams, fibers, and colloids, and that these materials exhibited a variety of interesting material properties, including high mechanical strength,

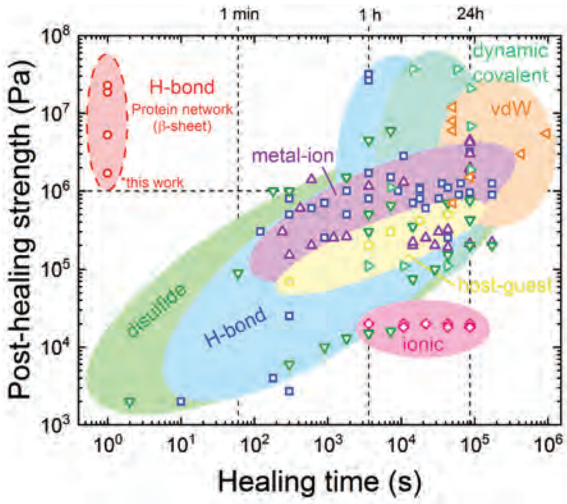

Figure 1: Performance of squid-inspired self-healing proteins ("this work," red oval, top left) compared to that of state-of-the-art self-healing materials that use different chemistries. This provides a benchmark for self-healing materials with respect to healing time (x-axis) and post-healing strength (y-axis). Adapted from Pena-Francesch et al. (2020).

thermal conductivity, and adhesive properties. Most significantly, Professor Demirel's early results emphasized a key tenet of biology—that sequence dictates structure and function. He found that the material properties could be tuned based solely on the sequence of the SRT protein that he used to create the material. Dr. McElhinny recognized the potential of this intriguing natural protein to sample a vast material property landscape while exploring the fundamental relationship among the protein sequence, structure, and material properties, and encouraged Professor Demirel to not limit his project to a single target material property. By creating large libraries of engineered non-natural variants of SRT protein, Professor Demirel could explore the material properties that become accessible when one controls the sequence of the protein. This research would also enable correlation of resulting material properties to protein sequence, laying the foundation for the rational design of protein-based materials with targeted properties.

RESULT

Professor Demirel and his team successfully developed a protein engineering methodology that enabled the synthesis of libraries of SRT protein variants with controlled length, which was a key challenge for this effort. SRT proteins contain tandem repeat sequences, which are inherently challenging to manipulate using traditional genetic engineering tools because repetitive sequences are prone to unintended duplication or deletion. Using this novel methodology, the team surveyed large libraries of novel proteins created by assembling repetitive sequences from SRT protein in different configurations, testing material properties including extensibility, stiffness, tensile strength, toughness, conductivity, optical transparency, and self-healing. From this analysis, in FY20, the team identified synthetic SRT-inspired proteins that demonstrated impressive self-healing capabilities relative to the current state of the art for soft synthetic polymeric materials described previously. The protein-based materials self-heal in less than 1 s and exhibit recovery of the original strength of the material post-healing (Figure 1). The self-healing protein-based material heals with the application of water and heat, although Professor Demirel is also considering approaches that could support self-healing triggered by light.

The team demonstrated rapid and robust self-healing in response to a variety of different types of mechanical damage, including scratches, punctures, and full severing of the material by cutting. Scratches were healed in less than 2 s, and punctures and cuts were healed in less than 1 s. As a demonstration of the high material strength recovered post-healing, which is a key limitation of current chemical-based self-healing approaches, material that is cut and then healed does not fail at the site of the healing, but at random locations that were not damaged or healed (Figure 2). The research team also produced a soft pneumatic actuator composed of the self-healing material and

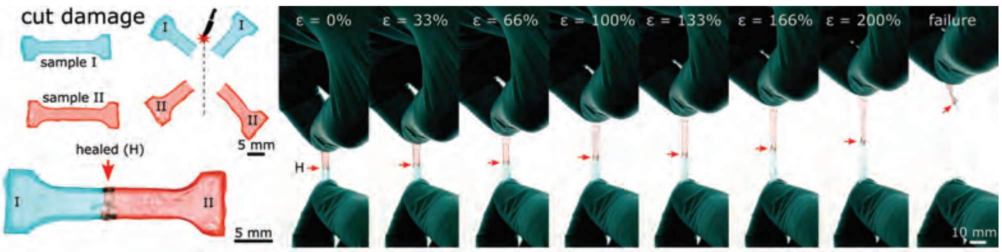

Figure 2: Total cut damage of dog-bone-shaped samples of protein-based material (I and II) that healed in less than 1 s. Healed samples withstood large deformations of up to 200% stretching strain before failure from a random pristine location, and healed areas were at least as strong as pristine areas. Site of healing is denoted by the red arrow. Adapted from Pena-Francesch et al. (2020).

ARL Competencies:

Sciences of Extreme Materials

Biological and Biotechnology Sciences

Results

- Generated an engineered protein capable of self-healing in less than 1 s, relative to current approaches that typically take 24 h or more.
- Demonstrated that the healed protein material recovers the strength of non-damaged material.
- Successfully engineered and identified a protein with superior self-healing properties, validating the potential of screening libraries of SRT-inspired proteins for new materials for Army applications.
- Garnered significant interest from ARL WMRD and DEVCOM CBC researchers who are now discussing potential transition opportunities.

Anticipated Impact

The self-healing protein-based material is expected to enable robust and reliable flexible polymeric materials that can undergo continual repetitive movement, which would advance capabilities of robotic machines, personal protective equipment, and prosthetics for the Army.

demonstrated a soft robotic system capable of gripping delicate objects and an artificial muscle that could repeatedly lift a dead weight at least 3,000 times heavier than its own mass. Moreover, these protein-based materials are 100% biodegradable into the same, original protein and can be triggered to degrade on demand by treating with an acidic solution. These results were published in *Nature Materials* in July 2020 (Pena-Francesch et al., 2020).

WAY AHEAD

These results illuminate the landscape of material properties that become accessible by going beyond proteins that exist in nature using synthetic biology approaches. The rapid and high-strength self-healing of these synthetic proteins demonstrates the potential of this approach to deliver novel materials for future Army applications, such as personal protective equipment or flexible robots that could maneuver in confined spaces. The potential of Professor Demirel's synthetic biology approach to access material properties that may be impossible to achieve through synthetic chemical approaches is of significant interest to ARL WMRD researchers, and Professor Demirel was invited to present a seminar on his research on November 5, 2020. In addition to continued research screening of the protein libraries for variants with desirable material properties under the ARO grant, Professor Demirel's team will also focus on opportunities to scale production of the self-healing SRT-inspired protein for future prototyping efforts. Dr. McElhinny has connected Professor Demirel with researchers at DEVCOM CBC to explore potential opportunities to scale production of the self-healing protein using the new DEVCOM CBC pilot-scale bioproduction facility.

This success was made possible by:

Dr. Stephanie McElhinny,
Life Sciences Branch

Citations:

Rabb, J. “Functional Redundancy Can Help Cells Balance Competing Biochemical Objectives,” *University of Colorado Boulder*. (2020).

Ruppe, A., Mains, K. & Fox, J. M. *Proc. Natl. Acad. Sci. USA* **117**, 23557-23564 (2020).

SUCCESS STORY

Tuning the Output of Biochemical Pathways Using Enzymes with Overlapping Functions

ARO-funded research devised the most complete model to date of the fatty acid synthesis pathway in the bacteria *E. coli*, revealing design rules that enable the fine-tuning of the products produced by a biochemical pathway. These findings reveal how genetic circuits could potentially be engineered in future cell-free systems to produce novel materials or fuels with a precision not possible using current manufacturing methods.

CHALLENGE

The metabolic pathways of bacteria are a remarkably optimized system of rapid and accurate catalysis that surpasses the speed and accuracy of most any manufacturing process, yet these natural pathways are restricted to produce only the biomolecules needed by the cell. The controlled output of engineered biochemical pathways remains an enduring challenge in the field of synthetic biology. Often the control schemes designed for engineered biochemical pathways do not effectively maintain production of the desired product(s) at a consistent level. This unreliability poses significant challenges for the field by hindering the demonstration of robust synthetic pathways supporting production of high-value molecules that could be scaled up to meaningful levels for commercial use. The prevailing approach to biological control of engineered pathway production focuses on transcriptional regulation—turning biochemical activities “on” and “off” by controlling the production of different enzymes. However, this approach does not support identification of the kinetic or structural relationships that allow enzymes to work together to perform nonlinear tasks, such as the iterative synthesis of polymeric products or the rapid (1-10 s) integration of chemical signals. These tasks remain difficult to design and control with the existing tools of systems and synthetic biology.

ACTION

In 2017, Dr. McElhinny received an initial inquiry from Professor Jerome Fox, an early career investigator at the University of Colorado Boulder. Professor Fox proposed an intriguing study to illuminate the importance of functional redundancy in biology—why biology would devote resources and energy to produce multiple biomolecules that appear to perform the same function? Professor Fox proposed that understanding why biochemical pathways utilize functional redundancy could explain how biological systems are able to perform complex, nonlinear tasks. Dr. McElhinny appreciated the significant potential of this research to provide a novel design tool for synthetic biology that would go beyond traditional transcriptional regulation approaches and would instead focus on the design of logic structures constructed via multi-enzyme pathways. In addition to the scientific innovation of Professor Fox's concept, Dr. McElhinny recognized that he would be a very strong candidate for the Presidential Early Career Award for Scientists and

Engineers (PECASE). She prepared a successful nomination package for the FY18 PECASE competition, and Professor Fox received an Army Early Career Award for Scientists and Engineers (ECASE) award in December 2018 (transition to PECASE pending approval by the White House).

RESULT

The objective of Professor Fox's ECASE project is to examine the design rules and logic structures that enable multi-enzyme systems to perform complex, nonlinear operations using the fatty acid pathway of *E. coli* as a model system. The fatty acid synthesis pathway was selected as an ideal model system to explore nonlinearity and emergence in biocatalytic networks for three key reasons: (1) this pathway builds fatty acids through an iterative elongation process that requires precise enzyme-level regulatory controls to tune both the length of fatty acids and their rate of production; (2) this pathway provides a biosynthetic route to an important set of oleochemicals (i.e., akyl esters, alkanes, alcohols, and polyhydroxyalkanoates for fuels, surfactants, and plastics) for which precise control over product profiles has proven difficult to achieve; and (3) the enzymes of this pathway can be isolated with ease, allowing experimental testing and validation of predictions made based upon the kinetic model. Professor Fox aims to systematically map biocatalytic processing in this pathway by reconstituting the fatty acid pathway outside of the cell to identify kinetically coupled controls and functional advantages of biocatalytic pathway branching to tune pathway output.

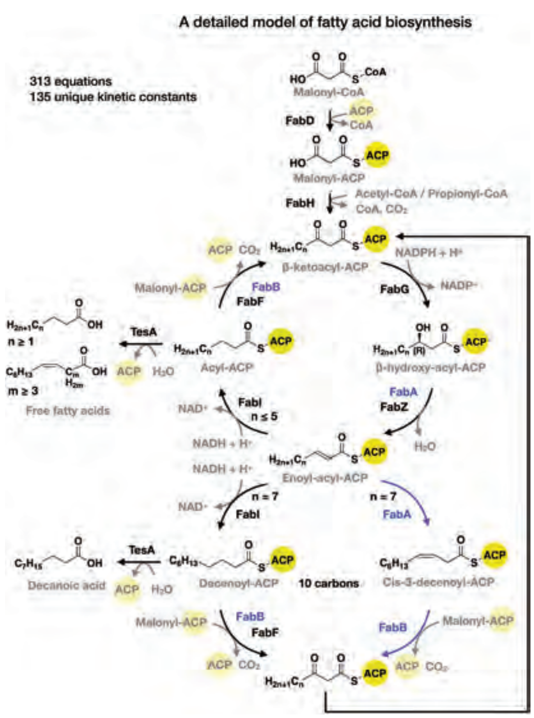

Figure 3: Kinetic model of the complete fatty acid synthesis pathway of *E. coli* comprising 313 equations and 135 unique kinetic constants. FabA and FabB specialize in the assembly of unsaturated fatty acids (blue), but also carry out several additional steps carried out by FabZ and FabF. The model captures the activities of all nine enzymes necessary to convert acetyl-CoA and malonyl-CoA to free fatty acids. Adapted from Ruppe et al. (2020).

In FY20, Professor Fox and his team developed the most complete model of the fatty acid synthesis pathway in *E. coli* to date, containing 313 equations and 135 unique kinetic constants (Figure 3). This model predicted that the ratio of different products produced could be tuned by simply controlling the ratio of enzymes with partially redundant functions within the pathway. This prediction was experimentally validated using the in vitro reconstituted pathway, indicating that partially redundant enzymes enable independent control over competing biochemical objectives. These results were published in September 2020 (Ruppe et al., 2020). Many biological systems have redundant components, but the importance of these components is rarely clear. These results help define the value of functional redundancy in a complex biochemical pathway and create a framework for carrying out similar analyses for other systems. These results also identify a novel control scheme for synthetic biology systems that avoids the need for engineered regulatory pathways that could be lost over time in cells.

WAY AHEAD

Professor Fox and his team will build on the results in three major ways in the coming years: (1) they will expand the detailed kinetic model of the *E. coli* fatty acid synthesis pathway to include the production of oleochemical products (e.g., alcohols, alkanes, methyl esters, methyl ketones, and polyhydroxyalkanoates for fuels, lubricants, flavoring agents, and plastics); (2) they will combine the kinetic model and in vitro experimental system to characterize and test different versions of the fatty acid synthesis pathway containing different combinations of wild-type and mutant enzymes; and (3) they will compare the model and *in vitro* predictions with in vivo behaviors in cells. This could help identify additional protein components that might be influencing performance of the pathway. Longer-term goals include testing the design rules elucidated by the kinetic model in other types of biochemical systems, such as bioluminescent systems.

ARL Competencies:

Biological and Biotechnology Sciences

Results

- Developed the most complete kinetic model of the fatty acid synthesis pathway in *E. coli* to date.
- Experimentally validated model predictions indicating that pathway output can be tuned by controlling the ratio of enzymes with partially overlapping function.
- Provided a framework for a novel control scheme for nonlinear tasks in synthetic biology systems that could potentially be engineered in future cell-free systems to produce novel materials or fuels with a precision not possible using current manufacturing methods.

Anticipated Impact

This research will reveal the biochemical basis of information processing, dynamic stability, and "low-power complexity" in living systems by answering the question, how do biological systems do so much with so little? The results are expected to enable the design and construction of dynamically adjustable biochemical systems that can perform complex tasks with minimal energy demand, such as photomimetic materials, stimuli-responsive bioluminescent displays, and rapidly adjustable biomanufacturing pathways.

GENETICS PROGRAM

Program Manager
Dr. Micheline (Mimi) Strand
Chief, Life Sciences Branch

Dr. Strand completed her undergraduate studies at Oberlin College, receiving her B.A. in Biology in 1985. She trained as a geneticist at the University of North Carolina at Chapel Hill, receiving her Ph.D. in Genetics and Molecular Biology in 1995. She trained for an additional five years as a postdoctoral fellow at the National Institutes of Health.

She came to ARO in 2000 as the Program Manager for Genetics.

Current Scientific Objectives

1 | Understand the molecular biology and genetics of mitochondrial regulation and biogenesis in order to, if successful, extend the ability of Warfighters to maintain peak cognitive and physical performance.

2 | Understand the regulation of free radical production and control in order to, if successful, reduce Warfighter senescence, injury, and death.

3 | Exploit genetic variation that, if successful, will create new sensing and intelligence capabilities.

This success was made possible by:

Dr. Micheline Strand,
Life Sciences Branch

Dr. Robert Kokoska,
Life Sciences Branch

Citations:

Moger-Reischer, R. & Lennon J. T. *Nat. Rev. Microbiol.* **17**, 679-690 (2019).

Smith, A., Parkes, M. A. F., Atkin-Smith, G. K., Tixeira, R. & Poon, I. K. H. *WikiJournal of Medicine* **4**, 8 (2017).

SUCCESS STORY

Aging, Senescence, and Death: The Impact on Warfighter Readiness

Aging and death have been traditionally studied in multi-celled organisms such as humans, mice, and fruit flies. Single-celled species such as yeast and bacteria, however, also age and die. Studies on aging and death in single-cell organisms yield new insights into the molecular mechanisms by which cellular and metabolic functions decline with age. These results have implications for extending the time that Soldiers remain fit for duty.

CHALLENGE

Staying alive is a matter of avoiding severe trauma (such as avoiding ballistics on the battlefield) as well as successfully maintaining cellular, organ, and organismal function in the face of an ever-increasing accumulation of damage to DNA, proteins, and organelles (visibly seen in humans who age out of being fit for duty or are too old to enlist in the Army). Until recently, longevity and aging had been studied in sexually reproducing multi-celled organisms, as single-celled organisms were erroneously thought not to senesce or die. Failure to survive and reproduce is an issue in the Army use of engineered single-celled organisms for synthetic biology or to produce biomaterials. Extreme success at surviving, such as *B. anthracis* cells that can reproduce when they are 100,000 years old, is also an Army problem. Finally, because experiments can be rapidly done on large numbers of bacteria that cannot be done on humans, new insights into human aging and senescence have emerged from studying aging in single-cell organisms.

ACTION

ARO is working to gain a fundamental understanding of how DNA damage accumulates in organisms over time; how patterns of DNA damage vary with environmental conditions; how organisms successfully or unsuccessfully avoid, repair, and mitigate DNA damage to both nuclear and mitochondrial DNA; and how such mitigating molecular pathways could be turned on or turned up in Soldiers. Warfighters are exposed to significant stressors, both physical and psychological, not normally encountered by civilians. These stressors can phenotypically express themselves in post-traumatic stress disorder (PTSD), suicide, organ failure, fertility issues, and other conditions that interfere both with Warfighter readiness as well as a successful post-service return to civilian life. Decoding patterns of DNA damage also has implications for developing new Army forensic and intelligence capabilities.

Dr. Strand and her ARO colleagues recognized the potential significance of investing in this type of research in 2012 and began investing then with Single Investigator (SI) funding. Results from the initial SI funding were promising and ARL investment was expanded to include Multidisciplinary University Research Initiative (MURI) funding in 2014. Key supported investigators include Dr. Michael Lynch at Arizona State University and Dr. Pat Foster at Indiana University.

RESULT

In general, larger organisms live longer than smaller organisms. A bowhead whale, which can weigh over 120,000 lb, can live over 200 years. A typical bacteria, on the other hand, only lives about two months. However, there are very interesting exceptions. Living bacteria have been extracted from permafrost, halite crystal, and amber that is millions of years old. While a typical microorganism in the lab can reproduce in 20 min, those living in the deep biosphere below the Earth's surface generally reproduce less than once a century.

Like in cars, damage accumulates in cells over time, leading to an ever-increasing probability of decreased performance and irreversible system failure (Figure 1). Damage accumulates in DNA in the form of single nucleotide mutations, insertions and deletions, recombination, and telomere shortening. This damage can be caused by normal intracellular processes such as energy production, protein synthesis, and protein recycling or by external agents such as ultraviolet light, ionizing radiation, and genotoxic chemicals. All organisms, no matter their size, face a tradeoff between reproduction and longevity; both require resource allocation and no organism has infinite resources. Longevity and the ability to reproduce can be extended by repairing the DNA damage directly through a number of different intracellular DNA repair pathways. Damage is also reduced by cell cycle arrest, where the cell stops reproducing and devotes itself to repairing the DNA damage before proceeding. In a resource-rich environment such a delay can lead to a competitive disadvantage. All cells must actively engage in removal of damaged proteins and failure to efficiently remove garbage is thought to contribute to aging-associated disorders such as Alzheimer's disease. Bacteria also dispose of garbage by aggregating it into minicells and

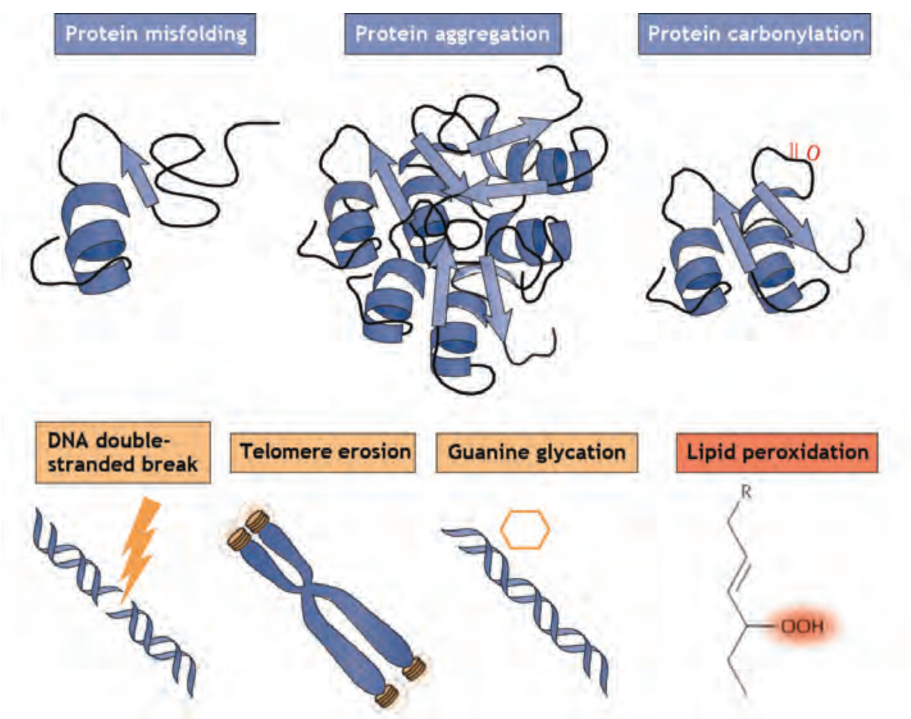

Figure 1: Example of types of damage to DNA, proteins, and lipids during aging. Because of the diversity of types of damage, it becomes impossible for the cell to repair them all, and damage accumulates as the cell ages. Figure and caption adapted from Moger-Reischer and Lennon (2019).

ARL Competencies:

Biological and Biotechnology Sciences

Results

- Gained a new understanding of how cells and organisms age.
- Identified new possible approaches for treating persistent infections.
- Identified new potential approaches for maintaining Warfighter readiness longer.
- Briefings given to and being followed by Army scientists for potential transition to intelligence applications and improved Warfighter health and protection.

Anticipated Impact

It is anticipated that this work will lead to better protection against natural or manmade infectious agents, particularly those that are resistant to normal therapeutics. It is also anticipated that these insights will, in the future, enable delayed senescence in Warfighters and civilians.

then removing them, similar to humans taking their garbage out of the house. In multicellular organisms such as humans, if a cell's damage becomes intolerable, it undergoes apoptosis, or programmed cell death (Figure 2). Although somewhat counterintuitive in a single-celled species, apoptosis also occurs in yeast cells that are irretrievably damaged, and elements of programmed cell deconstruction are also seen in bacteria. Finally, although the production of offspring phenotypically appears quite different in bacteria versus humans, bacteria also actively engage in sorting resources between mother and daughter cells: aging-associated protein aggregates and other undesirable elements are sorted into the mother cell, whereas the daughter cell starts life without most of the age-accumulated molecular garbage.

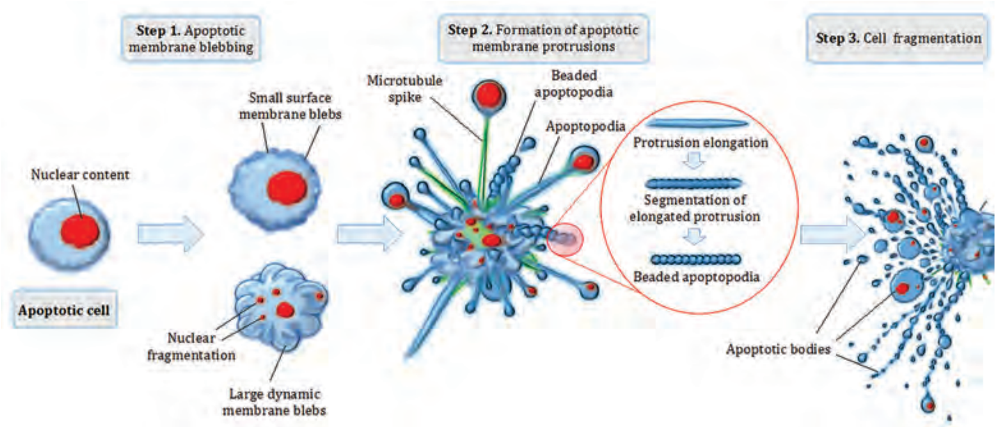

Figure 2: Apoptosis: cellular apoptosis is an active programmed process. Figure and caption adapted from Smith et al. (2017).

WAY AHEAD

Although these scientific advances support the hypothesis that individual humans will never be able to live forever, they shed light on molecular mechanisms that can be manipulated to slow aging-associated declines in human performance capabilities. Inducing programmed cell death in bacteria is a new approach and important for human health as resistance to currently available antibiotics continues to increase. Asymmetric distribution of aggregated and damaged proteins into daughter cells has recently been confirmed to also occur in mitotic replication in mammals. This selective segregation diminishes as humans age and this loss of selective segregation is likely to contribute to neurocognitive deficiencies. Finally, these results predict that aging, senescence, and death are universal; we may find life on Mars, but, like us, Martians won't live forever.

This success was made possible by:

Dr. Micheline Strand,
Life Sciences Branch

SUCCESS STORY

Mitochondrial Chromatin Accessibility

Chromatin accessibility in eukaryotes is regulated by a number of proteins that alter access in order to regulate gene expression in response to diverse conditions. Gene regulation is the mechanism by which a cell produces the set of proteins that are optimal to a specific set of intracellular and extracellular conditions. The work has prompted a phase shift in our understanding of mitochondrial gene regulation.

CHALLENGE

While chromatin accessibility in eukaryotes and nucleoid accessibility in prokaryotes is regulated by numerous proteins, data published to date has indicated the presence of only a single regulator in mitochondria, namely, mitochondrial transcription factor A (TFAM). Such simple regulation is somewhat unexpected as mitochondrial gene expression must closely coordinate with nuclear gene expression and cellular and organismal energetic needs.

ACTION

Dr. Strand had 14 years of research experience, including training as a graduate student and a postdoctoral fellow, and in the biotechnology industry, before coming to ARO. Based on her hands-on expertise in mitochondrial genetics research, she recognized that mitochondrial gene regulation

Understanding the agents that mutate mitochondrial DNA and the systems that repair or fail to repair those mutations, the regulatory systems that control which mitochondria and which mitochondrial genomes replicate, the factors that influence the rate of escape of free radicals from oxidative phosphorylation, and the regulatory systems and genes and proteins and genetic variants that affect mitochondrial function are critical for the Army to gain the capability to delay mitochondrial senescence in Warfighters.

is an area that is scientifically ripe for Army investment. Mitochondrial integrity and mitochondrial energy production capabilities are major drivers of both cognitive and physical performance capabilities. In general, aged mitochondria produce more free radicals and less energy, and are a primary (if unstated) reason that the Army generally enlists people in their 20s not people in their 60s. As a result of the scientific insights from her training, Dr. Strand identified several investigators that the Army should invest in, including Dr. Dan Mishmar at Ben-Gurion University of the Negev.

RESULT

Enabled by ARL extramural funding, Dr. Mishmar utilized new technologies to determine whether mitochondrial DNA accessibility was determined by more than TFAM, identify mitochondrial DNA variants that affected higher-order mitochondrial organization, and determine whether transcriptional regulation is modified in response to stress. Dr. Mishmar determined, using DNase I hypersensitive sites sequencing (DNAase-seq) and the assay for transposase-accessible chromatin using sequencing (ATAC-seq) experiments from both mouse and human samples, that mitochondrial DNA is organized into a higher-order structure that is influenced by signals from the nucleus and that this system is more complex than originally thought and involves more than TFAM.

WAY AHEAD

Dr. Mishmar and other investigators, with the support of ARO funding, will continue to work at the cutting edge of mitochondrial genetics and molecular biology to identify and elucidate the molecular factors that control the regulation of mitochondrial transcription and mitochondrial reproduction as well as those factors that affect mitochondrial integrity, energy output, and the release of free radicals. Mitochondrial integrity and function are essential for human life and Warfighter performance.

ARL Competencies:

Biological and Biotechnology Sciences

Results

- Published a peer-reviewed paper in *Frontiers in Genetics*.
- The principal investigator briefed Army and NASA scientists for potential transition to improve Warfighter and astronaut performance.
- Work being followed by Army scientists at DEVCOM SC for potential impact on preventing and treating PTSD.

Anticipated Impact

Understanding the agents that mutate mitochondrial DNA and the systems that repair or fail to repair those mutations, the regulatory systems that control which mitochondria and which mitochondrial genomes replicate, the factors that influence the rate of escape of free radicals from oxidative phosphorylation, and the regulatory systems and genes and proteins and genetic variants that affect mitochondrial function are critical for the Army to gain the capability to delay mitochondrial senescence in Warfighters. Delaying mitochondrial senescence will prolong the time that Warfighters remain fit for duty, provide more energy for the cognitive and physical activities required of Warfighters, and enable a better transition back to civilian life after the Warfighter has finished Army service. Mitochondrial function is also directly linked to PTSD, anxiety, depression, suicide, and traumatic brain injury, and as such, these results will also have direct impacts on Warfighter and civilian health.

MICROBIOLOGY PROGRAM

Program Manager
Dr. Robert Kokoska

Dr. Kokoska completed his undergraduate studies at Villanova University, receiving his B.Ch.E. in Chemical Engineering in 1978. He trained as a biochemist at Duke University receiving his Ph.D. in Biochemistry in 1995.

He came to ARO in 2006 as the Program Manager for Biochemistry. He has also served as the University Affiliated Research Center (UARC) Program Manager and has been the Microbiology Program Manager since 2014.

Current Scientific Objectives

1 | Discover the dynamics and communication mechanisms that drive robustness and function within bacterial communities that, if successful, are expected to lead to the effective design of microbial-based platforms for on-demand fielded material synthesis.

2 | Develop and test experimental strategies to better understand the physiology of complex microbial communities that, if successful, will provide reliable new platforms for the study of the human microbiome.

3 | Identify and characterize microbial metabolic programming under harsh environmental conditions that, if successful, will provide new approaches in the field of synthetic biology toward fielded living material systems.

This success was made possible by:

Dr. Robert Kokoska, ARO Life Sciences Branch

Citations:

Huang, W. *et al*. *Proc. Natl. Acad. Sci. USA* **117**, 10681-10687 (2020).

"Microorganisms in Parched Regions Extract Needed Water from Colonized Rocks: Interdisciplinary UCI-Led Team Is First to Demonstrate Long-Suspected Survival Strategy," *UCI News*. (2020).

SUCCESS STORY
Life on the Rocks: Microbial Survival in Desert Environments

ARO funding led to the discovery of new mechanisms enabling microorganisms to stay alive and even thrive in desert environments marked by a lack of water and excessively high temperatures. These insights will help enable the Army to reliably use these microbes for applications such as materials synthesis and power generation within this harsh environment.

CHALLENGE

The study of how microorganisms use resources to maintain their life, convert food to energy, and reproduce have traditionally been performed in laboratory environments where environmental conditions such as temperature, humidity, and light are well controlled and where food sources and water are both plentiful and likewise controlled. While these studies have led to an impressive level of understanding about microbial life and how those findings translate into how all living creatures sustain their viability, most microbes are found in environments where the conditions for growth are far removed from the ideal conditions replicated in a laboratory environment. In fact, microbial life is present in practically every habitat on this planet, including desert environments where the dry hot conditions force microorganisms to scavenge for water any way they can.

To understand the process of survival in desert environments, standard laboratory experiments in petri dishes with bountiful levels of nutrients do not faithfully replicate desert conditions, forcing one to go directly to the source of this life. For this, scientists need to identify microbial samples directly from their native environment; for desert-dwelling microbes, this means finding rock or soil samples from the desert that contain microbial life and then facing up to the challenge of how one can study the features of these microbes with the rock or soil itself as the source of microbial sustenance.

ACTION

At a 2016 ARL workshop on Bioenabled Materials Synthesis & Assembly that Dr. Kokoska helped organize, which included a session on biological systems that thrive in extreme environments,

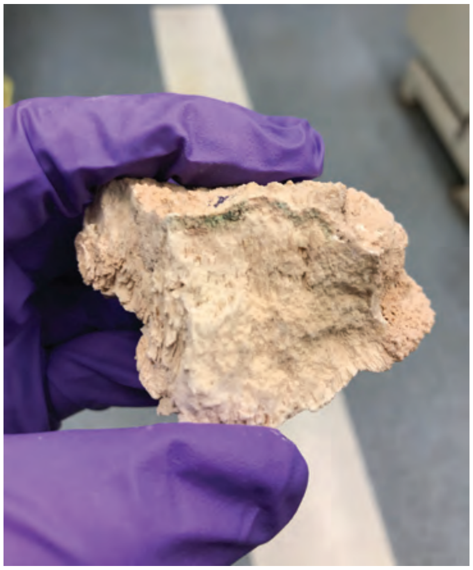

Figure 1: Researchers from Johns Hopkins University traveled to the Atacama Desert in Northern Chile to collect gypsum samples. Shown is a sample used to perform laboratory experiments to study the interactions between the gypsum and microorganisms present including the mechanisms by which the microbes extract water from the rock. Adapted from *UCI News* (2020).

Dr. Kokoska met with Professor David Kisailus of University of California, Irvine to brainstorm ideas and approaches by which one can effectively study microbial life under non-ideal conditions. With his background in material science, Professor Kisailus indicated that he was interested in collaborating with Professor Jocelyne DiRuggiero, a microbiologist at Johns Hopkins University who had recently retrieved gypsum samples from the Atacama Desert in Chile where she noticed bands of microbial growth in a thin layer below the surface of the gypsum that was protected from the environment's high levels of solar radiation and dryness (Figure 1), but the question remained: how were the microbes able to grow and colonize in this unusual environment?

Dr. Kokoska identified this scientific question as potentially groundbreaking and initiated a collaborative grant for these two investigators through the ARO Microbiology Program. Through this grant, Professor DiRuggiero was able to extract the microbes from these rocks and identified *Chroococcidiopsis*, a desiccation-resistant cyanobacteria found in many desert environments, as one of the primary microbial components. With Professor Kisailus working with intact gypsum samples, the team discovered that the presence of the cyanobacteria on the rock coincided with a phase transformation of the gypsum to a dehydrated material (Figure 2). This finding suggested that the microbes actually extracted water from the rock allowing for their colonization. To validate this, in a controlled experiment, the team allowed these microbes to colonize a rock sample under two different conditions: (1) in the presence of water, which mimics a high humidity environment, and (2) in a completely dry environment. They found that the phase transformation occurs only under the dry environment, where the microbes are stressed to the point where their only source of water was within the gypsum itself. Using advanced microscopy tools, Professor Kisailus observed that the microbes excreted organic acids when grown on the gypsum and discovered that these acids penetrated into the rock in specific directions within the rock crystal to more easily free up the water present between calcium and sulfate ions.

RESULT

This intriguing finding was the highlight of a publication in the *Proceedings of the National Academy of Sciences*, featured as a cover story of the May 19, 2020, issue (Huang et al., 2020). As this research sheds light on how living microorganisms can obtain and store water within stressful desert environments, it also encourages and motivates new thinking toward the discovery of other novel metabolic and cellular mechanisms that are required for maintaining life when there is a scarcity of other components such as carbon and nitrogen sources and essential minerals. Ultimately, uncovering these pathways will provide new evolutionary insights toward how life is sustained when stretched to extreme conditions and even encourage the development of new strategic ideas for how human performance can be maintained under similar conditions.

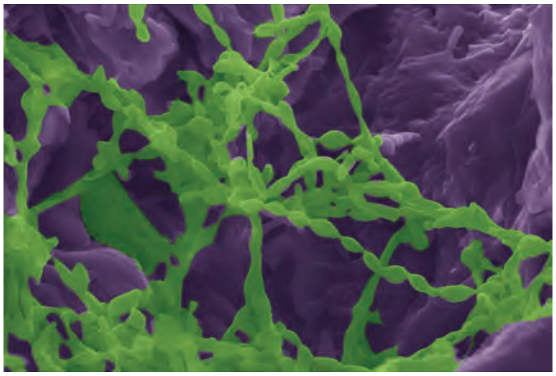

Figure 2: Scanning electron microscopy images that depict microorganisms (highlighted in green) colonizing gypsum sample (purple) from which water is extracted. Adapted from *UCI News*. (2020).

ARL Competencies:

Sciences of Extreme Materials

Biological and Biotechnology Sciences

Results

- Research resulted in the cover story in the *Proceedings of the National Academy of Sciences* May 19, 2020, issue.
- Led to reciprocal visits between ARL and Johns Hopkins University that have generated ideas that will support future academic–Army collaborations.

Anticipated Impact

Elucidating the mechanisms driving microbial survival in parched environments is expected to enable future enhanced leap-ahead technologies in the areas of field-based biomanufacturing and sensing.

WAY AHEAD

The Army has a strong interest in how microorganisms well adapted to extreme environments can be exploited for novel applications such as materials synthesis and power generation within these harsh environments. The results from this study and future follow-up studies focused on elucidating the metabolic pathways within these microbes responsible for the phase transformation in the gypsum will provide valuable clues for uncovering the evolved design strategies used by native desert-dwelling microbes to maintain their viability in the face of multiple environmental challenges. As such, scientists from the ARL's Transformational Synbio for Military Environments (TRANSFORME) Essential Research Program visited Professor DiRuggiero's laboratory at Johns Hopkins University in April 2019 and learned that there can be great synergy between the ARO-funded research and the goals of the ERP. Subsequently, Professors DiRuggiero and Kisailus visited ARL in February 2020 to give a seminar to ARL ERP scientists across Directorates to further brainstorm areas of potential collaboration.

This success was made possible by:

Dr. Robert Kokoska,
Life Sciences Branch

Citations:

Charubin, K., Modla, S., Caplan, J. L. & Papoutsakis, E. T. *mBio*. **11**, e02030-20 (2020).

Stewart, J. "When Two Bacteria Become One: Researchers Uncover How Microbial Cells from Two Different Species Combine to Form Hybrid Cells," *University of Delaware*. (2020).

SUCCESS STORY

Resource Sharing via Microbial Fusion

This ARO-funded initiative revealed a new mechanism by which different bacterial species fuse together to cooperatively share and exchange their genetic material and metabolites to perform functions that neither can perform individually. This unprecedented finding will provide the Army with new strategies by which microbial communities can be engineered and utilized for a broad range of biosynthetic processes.

CHALLENGE

Microbial life exists in practically every habitat on this planet. Beyond this, there is a rich diversity of hundreds, sometimes thousands, of different naturally selected microbial species that are part of a given ecosystem that collectively contribute to nutrient cycling and a "food chain" for all life in that habitat. As in human communities, individual members of these microbial communities will invariably share some of their resources and metabolites with other members of the community in order to help all members of the "neighborhood" sustain themselves. As there are numerous well-documented examples of this phenomenon of inter-species microbial metabolite sharing (termed syntrophic interactions), in considering the presence of hundreds of different microbial species in any given environment, a challenging scientific question has always been, how does a given species effectively find the right cooperative neighbor with whom to interact? In addition, what are the mechanisms by which this cross-feeding occurs in a way that is efficient enough to promote mutual growth?

ACTION

In October 2016, Dr. Kokoska was invited to speak at a workshop on Microbial Electrosynthesis sponsored by the Naval Research Laboratory (NRL) and the Advanced Research Project Agency – Energy (ARPA-E). During that workshop, he recognized the Army relevance of the research of Professor Eleftherios (Terry) Papoutsakis of the University of Delaware. Professor Papoutsakis presented his work on the cooperative relationship between two species of the bacterial genus Clostridium where *C. acetobutylicum* (*Cac*) feeds off of environmentally provided carbon sources providing reducing equivalents and carbon dioxide (CO_2) to support the growth *C. ljungdahlii* (*Clj*), which in turn, provides organic substrates back to *Cac* to drive its own metabolism. Remarkably, both species grown together synthesize organic compounds that neither can produce individually. Dr. Kokoska engaged with Professor Papoutsakis to learn more about his research, at which point, Professor Papoutsakis displayed some unpublished work that included an intriguing series of transmission electron micrographs showing that in co-cultures of *Cac* and *Clj*, individual cells between the two species invade each other; they are physically fused between their respective

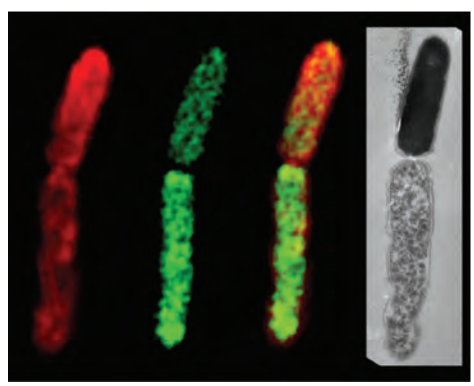

Figure 3: Fluorescence super-resolution structured-illumination microscopy (SR-SIM) imaging of a cell fusion event between green-labeled *C. acetobutylicum*-FAST (*Cac*) bound to a 4-hydroxy-3-methylbenzylidene-rhodanine (HMBR) ligand and red-labeled *C. ljungdahlii* (stained with CellTracker Deep Red) showing reciprocal diffusion of stained proteins between species. Far right: correlative transmission electron microscopy (TEM) image reveals ultrastructure of the fusion event at each of the cell poles. *Cac* is distinguished from *Clj* by the vegetative homogeneous texture of *Clj*. Adapted from Charubin et al. (2020).

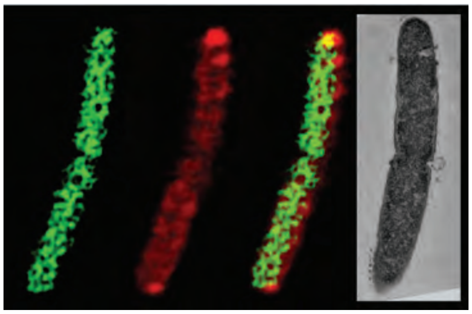

Figure 4: Formation of hybrid bacterial cells. Correlative SR-SIM imaging of hybrid *Cac-Clj* cells undergoing division. Individual species are stained as in Figure 3. Both cells display equally distributed red and green fluorescence. Correlative TEM image on the right shows that ultrastructure of both cells appears to be a hybrid of the two species. Adapted from Charubin et al. (2020).

cell membranes and cell walls. What makes this observation all the more interesting is that no such fusion events were observed between two cells of the same species, suggesting that the interspecies joining may provide a functionally efficient means for the two species to share metabolites.

As a means of quickly testing the hypothesis that these cell fusions do provide a means for metabolite exchange, Dr. Kokoska provided a 9-month grant to Professor Papoutsakis under ARO's Short-Term Innovative Research (STIR) Program. The results from this short-term study did in fact demonstrate that direct transfer for reducing equivalents from *Cac* to *Clj* and the novel synthesis of compounds that occur only in co-culture requires that the two species be in close proximity to each other, suggesting that cell-to-cell contact is required for the syntrophic interactions. To explore this further, Professor Papoutsakis wished to investigate whether interspecies joining can facilitate exchange of other larger biological macromolecules. Through a Single Investigator grant funded through the ARO Microbiology Program, Professor Papoutsakis demonstrated, through a series of rigorous experiments and an elegant use of fluorescence microscopy, that proteins and genetic material, in the form of ribonucleic acid (RNA), are indeed exchanged between the two species through their fused membranes (Figure 3). As proteins and RNA control cellular metabolism and gene expression, these fusion events result in a loss of individual identity of the two species. Curiously, some of these hybrid cells also continue to divide and can differentiate as spores containing the fused contents of each species (Figure 4). The ability of these two species to form functional hybrids in co-culture suggests a mechanism by which microbes within a community enhance their ability to survive. These findings can now also point to a new line of thinking in the field of microbiology to study metabolic processes that takes into account the sharing of genetic material and the control of numerous cellular processes conferred by the sharing of proteins with distinct functions from the "parent" species.

RESULT

This unprecedented finding of the exchange of proteins and genetic material between two different microbial species through a physical fusion event was published as an Editor's Choice in *mBio*, a journal of the American Society for Microbiology, in September 2020 (Charubin et al., 2020). These findings have the potential to impact many other studies in the field of microbiology and microbial ecology. This study was focused on cellular fusion between syntrophic species of Clostridium; as there are countless instances of interspecies cooperation in the microbial world, there is almost certain to be many other examples of physical cellular fusion as a more general mechanism that drives metabolite and macromolecular sharing between species, which will enhance our understanding of the factors that drive microbial evolution. In addition, the ability to engineer fused microbial species to generate new metabolic capabilities in hybrid cells would represent an exciting new capability in the field of synthetic biology. These findings can also impact human health as proteins that confer antibiotic resistance to certain strains of bacteria may also be shared with other species by this mechanism to enhance their own resistance. Also, these results could help provide an explanation for why individual species or strains of bacteria found in unique environmental niches are so difficult to culture or grow for studying their metabolism. There may be a direct dependence on other neighboring bacteria and their metabolic output. Thus, if other such fused pairings can be identified, we could devise effective strategies for culturing individual strains.

WAY AHEAD

The ARL Biotechnology Branch (ARL SEDD) has a keen interest in developing biological processes that can direct the conversion of field waste to either energy or commodity biochemicals. Since the metabolic capacity of some Clostridium species render them effective for the conversion of carbon-based waste material, the Army has a direct interest in fully understanding the metabolic consequences of interspecies fusion in order to develop effective design strategies for the targeted use of these species. Should a similar fusion phenomenon exist for many other microbial pairings, these findings will have a huge impact on our understanding of the human microbiome, which typically consist of hundreds of different microbial species, where there are numerous syntrophic interactions. This will certainly influence the interests of DEVCOM SC and the U.S. Army Research Institute of Environmental Medicine in the study of how nutritional input affects the activity of the gut microbiome and its downstream effects on cognition and human performance.

ARL Competencies:

Energy Sciences

Biological and Biotechnology Sciences

Results

- Discovered a new mechanism for information exchange between bacteria, which will impact our fundamental understanding of microbial evolution and the interactions that drive microbial community function.
- Research resulted in the September 2020 *mBio* publication as Editor's Pick (Charubin et al., 2020).

Anticipated Impact

The discovery of interspecies bacterial fusion is expected to enable future applications for the Army including in-field biological sensing, waste remediation, and biosynthesis.

NEUROPHYSIOLOGY OF COGNITION PROGRAM

Program Manager
Dr. Frederick D. Gregory

Dr. Gregory completed his undergraduate studies at Morehouse College, receiving his B.S. in Biology in 1999. He trained as a neurobiologist at the University of California Los Angeles, receiving his Ph.D. in Neurobiology in 2006.

He came to ARO in 2012 as the Program Manager for what was then called the Neurophysiology and Cognitive Neuroscience Program and then took on the additional role of International Program Manager for Human Dimension in 2016.

Current Scientific Objectives

1 | Map, measure, and model the structural and functional components of multisensory perceptual processes in the brain that, if successful, may lead to the capability of developing future non-invasive neurotechnologies that allow us to modulate human multisensory information processing bandwidths beyond normal ranges that can then be used, for example, to reduce cognitive errors in fatigued Soldiers.

2 | Determine how the brain structures, processes, and refines biological neural networks to generate efficient decisions and behaviors, while demonstrating robustness to injury that, if successful, will enable a deep understanding of multiscale neural phenomena, which will have potential future applications to maintaining peak cognitive performance and ensuring that the deleterious effects of traumatic brain injury and post-traumatic stress disorder (PTSD) can be mitigated.

This success was made possible by:

Dr. Frederick Gregory,
Life Sciences Branch

Citations:

"Airport Scanner 2," *Kedlin Entertainment*. (2018).

SUCCESS STORY

Applying Big Data to Enhance Human Visual Search Performance

ARO-funded research has led to discoveries of new ways to understand and improve expert human visual search skills that have transitioned to ARL. This new Big Data approach also resulted in the launch of a startup company that has begun to identify and help train real-world searchers working in transportation security around the world.

CHALLENGE

Visual cognition involves the processes of visual memory, perception, and attention, which underlies performance of visual search—the Army-relevant skill of finding potential targets among non-target distractors. Many Army jobs require Soldiers to perform complex visual search tasks, which may pose significant cognitive demands that can lead to life-or-death errors. Unfortunately, the best methods for training an individual's visual and attentional abilities more efficiently and effectively have not yet been determined.

ACTION

Dr. Stephen Mitroff's (George Washington University) earlier ARO-funded work focused on identifying different traits associated with better search performance. Working with a variety of expert groups, including airport security officers and radiologists, has helped the lab to explore and understand the effects of expertise and experience on visual cognition. Dr. Mitroff and his research team discovered new insights on a range of important topics, including how search performance is worse when more than one target is present, why some people are better able to search than others, and more. A few years ago, Dr. Gregory conducted a site visit to the Mitroff Lab. They discussed how this and other findings could be connected to potential strategies for identifying the best-suited individuals for jobs requiring intense search tasks. This discussion led to the idea of a workshop that would enable horizon scanning and input from multidisciplinary viewpoints focused on expanding the possibilities of future impacts from studying visual search processes in humans.

Figure 1: The Airport Scanner 2 game logo. Image reprinted from The Kedlin Company (2018).

Dr. Mitroff took on the challenge, and competed for and was awarded an ARO Conference and Symposia Grant to host the *Conference on Visual Search: A Comprehensive Treatment of Search* in December 2013. The two-day workshop included 18 speakers that covered a range of topics, including scene segmentation, clutter and camouflage, computational vision, and Big Data. Program officers and researchers from 13 funding agencies attended and contributed greatly to the discussions about how multidisciplinary collaborative work can greatly advance the study of visual search. Suggestions from that workshop included ideas like the field had to move beyond using artificial search tasks ("T"s and "L"s on a computer screen) as the major approach. This idea related to the need for more research involving search for more realistic targets in natural, dynamic scenes. Dr. Mitroff drew inspiration from the workshop outcomes and competed for follow-on funding in 2016.

RESULT

Dr. Mitroff's research since then has centered on an innovative direction—using "Big Data" as a research tool. Airport Scanner (Figure 1) is an app in which the player serves as an airport security officer and attempts to detect illegal and rare items in bags. Dr. Mitroff partnered with the creators of Airport Scanner to gain access to anonymous user performance data. This gives him the capability of designing impactful experiments based in the game that could be conducted right alongside traditional laboratory experiments. This dual approach offers a unique testbed for validating various hypotheses about skilled visual search performance. As of now, there are 3.79 billion unique trials from 15.47 million individual players. The Army could never afford to pay people to generate this much performance data. As a result, the pivot toward anonymous Airport Scanner user data has led to fruitful outcomes. When Dr. Mitroff presented his work to ARL scientists, they discussed the possibility of working together to support the Continuous, Multi-Faceted Soldier Characterization for Adaptive Technologies program effort to understand sources of human variability. Now, ARL is working together with Dr. Mitroff's team on a new collaborative research effort. The goal of this new research is to use Big Data as a tool to address the potential challenges that human variability will create if the Army intends to deploy teams of humans and autonomous agents in the future. Future autonomous teammates will need to interpret and adjust to the multiple states that we undergo during job performance, such as getting tired in the moment or changes in our level of expertise over time.

In addition to research, Dr. Mitroff's work has led to other outcomes that have benefited the Army. A new company, Kedlin Screening International (KSI), has been created to transfer technology from the Mitroff lab. KSI uses a brief visual search mobile application to inform personnel hiring, assessment, and training. So far, KSI is helping to screen and train superior search skills for transportation security agencies around the world, which can be adapted to enhance the proficiency of Army searchers as well.

An additional product from Dr. Mitroff's efforts has been scientific talent. Two postdoctoral researchers in the lab came to work for the DoD. One postdoctoral fellow became an active duty officer and is leading research, first, for the Navy Medical Research Unit in Dayton, Ohio, and now for the Naval Special Warfare Command. Another trainee came to work for the Army, spending several years at DEVCOM SC working as a civilian scientist. Two postdoctoral researchers also successfully competed for their own complementary ARO funding to lead independent projects while still in the Mitroff Lab. One of those projects explored visual search in a video game environment that allowed exploration of how brain training may help to avoid civilian casualties by friendly fire. Both projects received ARO Short-Term Innovative Research (STIR) funding, which provides an excellent opportunity to highlight new concepts and explore new basic research areas. These postdocs were able to establish their research independence and develop a strong foundation for their careers. Overall, this project has brought some of the best and the brightest minds to work for the DoD as well as leading to impactful Army-relevant discoveries.

ARL Competencies:

Humans in Complex Systems

Results

- Results of his team's ARO-funded projects appeared in over 40 peer-reviewed academic publications and over 100 academic and industry presentations.
- Provided in-house expertise in an area of high Army-relevance, as two of Dr. Mitroff's trainees have come to work for the DoD.
- The Airport Scanner massive dataset transitioned into an active collaboration with ARL, which will enable the Army to train Soldiers to be their best for any mission requiring exceptional visual search cognition and awareness, like breaking camouflage.

Anticipated Impact

Further collection and analysis of Airport Scanner data, combined with integration to laboratory studies, will enable DEVCOM to advance modeling of human performance and accelerate understanding of human variability's impact on Soldier performance as the Army faces the challenge of preparing for future Multi-Domain Operations.

WAY AHEAD

Dr. Dwight Kravitz, a co-investigator and associate professor at George Washington University, is working with Dr. Mitroff to use the Airport Scanner data to pursue timely and critical evaluations of broader data analysis practices used in research. In addition to the commercial applications for transportation security, this immense dataset provides an exciting testbed for investigating the impact of seemingly simple research design choices. The research team will next attempt to understand the contribution of different sources of statistical variance (e.g., human variability, implicit learning of the environment) in order to build better models of human cognitive performance. This effort will be facilitated by the ongoing partnership between Dr. Mitroff's team and ARL.

This success was made possible by:

Dr. Frederick Gregory,
Life Sciences Branch

Dr. Virginia Pasour,
Mathematical Sciences Branch

Citations:

Levinthal, D. J. & Strick, P. L. *Proc. Natl. Acad. Sci.* USA **117**, 13078-13083 (2020).

"Research Shows Connection between Stress, Stomach Ulcers," *DEVCOM ARL Public Affairs*. (2020).

SUCCESS STORY

Understanding Gut Feelings: From Gut to Brain and Back

New ARO-funded research identifies, for the first time, how multiple regions of the cerebral cortex influence the stomach via the vagus nerve and its numerous pathways. This work points out brain-to-gut connections that might underlie how post-traumatic stress disorder (PTSD) controls the composition of microbes in the gut and supports the old adage of treating PTSD with "three hots and a cot" due to the observed gut-to-brain targets.

CHALLENGE

Scientific studies over decades have identified the psychological profiles and psychophysical advantages afforded to experts in many fields of sports and the arts when they performed, compared to novices. Results of these efforts led to popularization of concepts such as "being in the zone" and the "10,000-Hour Rule," claiming that world-class expertise in any skill requires around 10,000 h of deliberate practice. The uprising of functional magnetic resonance imaging in the late 1990s and early 2000s led to hundreds of studies that sought to identify features of expert's brains that afforded advantages over the rest of the population. Comparisons showed correlations between metabolic changes in brain regions associated with controlling motor and sensory functions involved in the skilled performance as well as other regions associated with the decisions to act. Around this time, there was also a revolution in the understanding of cellular and molecular mechanisms underlying learning and memory. By the early 2010s, a large body of evidence pointed to synaptic plasticity as the candidate mechanism for mediating all learning and memory. These bodies of work naturally identified synaptic plasticity as a vital component of learning to become an expert, but there remains a gap in understanding how synaptic plasticity (at the cellular scale) enables mind–body control of expert performance (at the systems and organism level). This lack of understanding phenomena across size scales is a general impediment in neuroscience and limits the extent to which neuroscience will directly impact Army human sciences challenges associated with accelerated learning for a ready and responsive force. Is the "10,000-Hour Rule" a biological necessity? Can neurophysiology generate an opportunity to reduce the amount of time it takes to train expertise for military-relevant tasks? ARO initiated actions, beginning in 2014, to address these outstanding questions by exploring opportunities for Army research and strategic extramural basic research. Those actions laid the groundwork for recent findings that are leading to deeper insight into the extent to which the "gut feeling," which we all understand, may be a vital component of the brain's journey when we gain expertise.

"The stomach sends sensory information to the cortex, which sends instructions back to the gut. That means our 'gut feelings' are constructed not only from signals derived from the stomach, but also from all the other influences on the rostral insula, such as past experiences and contextual knowledge."

– Dr. Peter Strick, University of Pittsburgh

ACTION

To identify grand challenges for the Army of 2050, ARO Neurophysiology of Cognition Program Manager, Dr. Frederick Gregory, co-organized the Human Dimension Basic Research Concept Exploration meeting for ARL. The meeting enlisted the expertise of an academic panel to identify research gaps in quantifying human behavior, and other topics in cognitive sciences that included training expertise. The conclusions, published in the 2014 Army Science Planning and Strategy Report, included a recommendation that the Army should invest in multidisciplinary studies to enhance education and training for optimal decision-making. As a result, Dr. Gregory identified fundamental scientific barriers that must be addressed to augment skill learning. The state of the art in psychology, neuroscience, human factors, and human performance typically compared an independent variable between a group of novices and a group of experts.

After hundreds of journal articles identifying correlative relationships between a study's independent variable and performance, conclusions emerged that expertise is mediated by distinct changes in the structure and function of the brain. In 2014, Dr. Gregory explored the potential for a new multidisciplinary approach to identify brain and body state variables that transition as an individual journeys from novice to expert. In 2015, the Executive Director of the National Institute for Mathematical and Biological Synthesis (NIMBioS) was interested in this idea and invited Dr. Gregory and the ARO Biomathematics Program Manager Dr. Virginia Pasour to propose a cutting-edge workshop to address the scientific challenges associated with understanding expertise. As a result, they identified key researchers in the field and initiated the 2015 Neurobiology of Expertise investigative workshop. The meeting brought together leading mathematicians, neuroscientists, and psychologists. This included the psychologist whose research led to coining of the "10,000-Hour Rule."

Drs. Gregory and Pasour leveraged the results from the workshop to devise a novel multidisciplinary basic research challenge. They identified that a major aspect of physical expertise involves seamless decision-making and control of the stress response, and formulated a Multidisciplinary University Research Initiative (MURI) topic to define expertise by discovering the underlying neural mechanisms of decision-making during skill learning. The MURI topic was one of the eight ARO topics selected for public release in the FY16 MURI Broad Agency Announcement. Dr. Scott Grafton's proposal from University of California, Santa Barbara was awarded in late 2016. The focus on learning expertise in a decision-making task combined with experimental and theoretical approaches from psychology, neuroscience, network sciences, and mathematics was an ideal approach to develop a novel multiscale modeling framework to identify causative neural and physiological mechanisms. Together, a suite of experimental and analytical tools are used to probe and model similar decision processes in human, non-human primates, and rodents, since they all show similarly involved brain structures, learning processes, and behaviors.

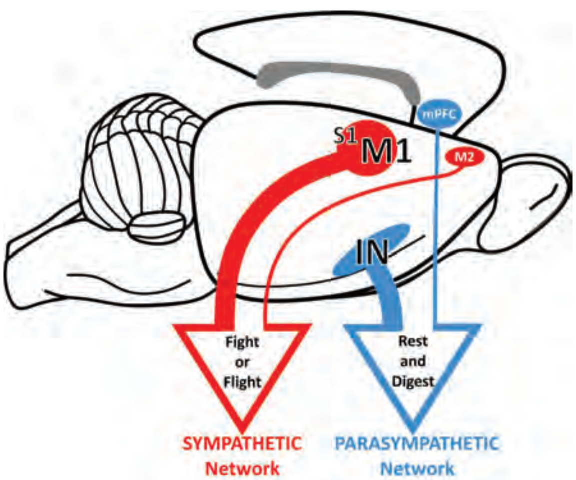

Figure 2: Distinct brain networks influence parasympathetic and sympathetic autonomic control of the stomach. Adapted from Levinthal and Strick (2020).

RESULT

In addition to looking at the brain, this team also looked to the body. A fundamental aspect of expert performance is that the mind and body are focused effortlessly on executing the learned task. Recent experimental results in non-human primates from the University of Pittsburgh tracked specific neuronal pathways from the gut all the way to multiple sites in the brain involved in decision-making, memory, and emotions as well as sites implicated in neurological disorders like anxiety and PTSD (Figure 2).

In the broader context of expert performance, these preliminary results combine with other MURI team findings to chart a path toward understanding the neural basis for the brain and body changes that occur when one learns to become an expert and will inform strategies for regulating these processes to accelerate learning in future military training.

WAY AHEAD

This scientific accomplishment lays a foundation for uncovering underlying bases of human decision-making by strengthening the potential to translate information from primate behavioral tests, brain states, and computational models to human data. This research may ensure fidelity of future synthetic training environments by offering novel biomarkers and mechanistic understanding that will help optimize training of decision accuracy.

ARL Competencies:

Humans in Complex Systems

Results

- Discovered the anatomical basis for innervation of the stomach by the autonomic nervous system and has traced the pathways up to the brain.
- Provided the groundwork for addressing the basis of physiological modifications that accompany expert performance (i.e., emotion/stress regulation and focus).

Anticipated Impact

This discovery is expected to enable future leap-ahead technologies involving humans in systems such as accelerating learning in synthetic training environments.

SOCIAL AND BEHAVIORAL SCIENCE PROGRAM

Program Manager
Dr. Lisa Troyer

Dr. Troyer completed her undergraduate studies at the University of Washington, receiving her B.A. in Sociology in 1989. She trained at Stanford University, receiving her Ph.D. in Sociology in 1995.

She came to ARO in 2013 as a Scientific and Engineering Technical Advisor to support development of programming in the social and behavioral sciences. In 2015, she was appointed as Program Manager of the Social and Behavioral Science, Life Sciences Branch. Prior to joining ARO, Dr. Troyer served for 17 years as tenured Professor, Associate Provost, and Chief of Staff to the President at three Carnegie-classified Research I universities and consulted for several Fortune 500 organizations.

Current Scientific Objectives

1 | Identify and validate measurement methods to detect shifts in human behavior and collective action that, if successful, will lead to new tools to identify emergent conflict, violent extremist individuals and groups, and deception attempts by adversaries.

2 | Generate and validate predictive approaches to causally model emergent risks across individual, collective, organizational, and state levels that, if successful, will provide decision makers with improved operational effectiveness for early identification of emergent security risks at these different levels.

3 | Investigate interdependencies among social, natural, and physical systems to determine the spatial and temporal evolution of dynamics in these systems that, if successful, will enable long-range prediction of precursors of conflict and enable early prevention and mitigation strategies.

This success was made possible by:

Dr. Lisa Troyer, Life Sciences Branch

Citations:

Kalkhoff, W. *et al. SPQ* **83**, 26-48 (2020).

Melamed, D., Kalkhoff, W., Han, S. & Li, X. *Socius* **3**, 1-10 (2017).

SUCCESS STORY

Path-Breaking Research Identifies Neurological Indicators of Dominance and Social Influence in Groups

These investigations discovered neurological signals that indicate the evolution of dominance hierarchies in groups. The new capability to track this evolution is enabling innovative methods to identify group members who are likely to become most influential in groups, providing new capabilities to enhance Soldier lethality by increasing efficiencies in how groups are organized as leaders and followers, as well as determining potential leaders of friendly and adversarial groups to improve Warfighter overmatch.

CHALLENGE

It has long been recognized that groups rapidly develop a social hierarchy of dominance and influence, whether based on formal designations (such as relative rank, assigned leadership designations) or demographic characteristics (such as age, race, and gender associated with status), or when initially there are no observable differences that differentiate group members. As individuals rapidly become sorted into a hierarchy that hierarchy operates with remarkable efficiency to determine who influences whose decisions and behaviors and who defers to others, leading to highly coordinated collective action that enables the rapid achievement of commonly held goals. Sometimes, however, the hierarchies are challenged as members who are not designated leaders attempt to exert influence. This can create inefficiencies and emergence of unanticipated influential group members. Tracking the emergence of the hierarchy—who will become the dominant and influential group members, and how dominance contests emerge and are resolved—has been elusive. At best, scientists could simply observe the group over time and construct the social hierarchy after it had crystalized. What has been missing until ARO began to invest in solving this scientific puzzle are methods to track, in real time, how the hierarchy and influence are developing.

ACTION

Based on her professional leadership experience as a journal editor and elected leader of professional groups in the field of social psychology, Dr. Troyer became aware of innovative researchers working to advance the use of neural pattern tracing based on functional magnetic resonance imaging (fMRI) and electroencephalogram (EEG). Starting in 2015, she contacted researchers who might be able to apply these technologies to determine if there was potential for using them to track the emergence of dominance and influence hierarchies and the rise of dominance contests. Two scientists emerged with promising white papers from a pool of potential researchers: Dr. David Melamed (The Ohio State University) and Dr. Will Kalkhoff (Kent State University). The scientists agreed to work together, but develop independent proposals to work on these problems under Dr. Troyer's guidance, which she subsequently selected for investment. Dr. Melamed would focus on fMRI methods and models to examine differences in neural patterns in pre-established dominance hierarchies; Dr. Kalkhoff would tackle how EEG signals could be used to measure ambiguous dominance hierarchies that arise when expectations about who is most dominant and influential are violated, leading to the onset of dominance contests.

RESULT

Dr. Melamed's team developed an innovative experimental protocol that could be administered in an fMRI environment. The protocol entailed manipulating the status of group members prior to exposure to a decision-making task in which they would ostensibly receive feedback on the responses of others before making a final decision. The measure of influence is the frequency with which they adjusted their initial decision when other group members indicated an alternative decision. This was the first time this had been attempted in an fMRI setting that would enable study of brain region activity based on blood oxygenation-level dependent (BOLD) responses. Based on prior research, Dr. Melamed hypothesized that the nine regions of interest (ROIs) would most likely be those associated with dominance and influence dynamics, and found that five showed significant BOLD responses in the experiment: the dorsolateral prefrontal cortex (DLPFC), amygdala, thalamus, fusiform gyrus, and intraparietal sulcus (IPS). Importantly, the BOLD analyses showed that when dominance hierarchies are pre-existing (e.g., based on rank or leadership assignment), these ROIs were activated for less-dominant actors, indicating that they were attending to the input of the higher-status actors to solve the decision task, but not for the dominant actors. The results were published in *Socius* in 2017 (Melamed et al., 2017).

Dr. Kalkhoff's team collaborated with Dr. Melamed, recognizing that fMRI is suited for studying unconscious processing that may underlie subjective experiences of dominance and influence but may miss rapidly occurring patterns. EEG, in contrast, has high, millisecond-level temporal resolution, making it a promising approach for detecting the unconscious rapid formation of expectations about self and others that form the foundation for influence. An added advantage is that it is less intrusive than fMRI, and as the technology advances, may eventually enable non-intrusive means of detecting neural patterns, such as emergence of influential group members. Dr. Kalkhoff adopted a similar protocol to Dr. Melamed's to enable comparisons, but included conditions where influence expectations were violated (i.e., higher-ranking members' influence was ostensibly ignored; lower-ranking members' influence was adopted). This is akin to a dominance contest in which individuals who have been privileged by, for example, rank or other characteristics, anticipate influencing others but are denied that influence. Based on prior research, the Kalkhoff team recognized that the alpha frequency band (8-12 Hz) is prominent in

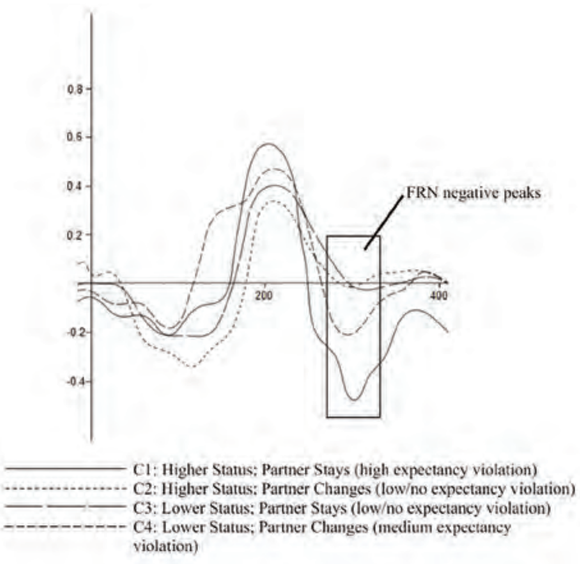

Figure 1: The waveforms-by-condition graph shows the evolution of brain activity, drawing attention to the FRN, demonstrating the negative amplitude peaks occurring at about 300 ms that are clearly differentiated when dominance contests occur. Adapted from Kalkhoff et al. (2020).

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

Results

- Discovered new neural signals of dominance and influence dynamics that are part of a broader ARO thrust on the biophysiological signals of emergent social dynamics.
- Transitioned findings to AFC's Directorate of Intelligence and Security (DoIS) through virtual seminar presentations.

Anticipated Impact

Identifying the underlying neural patterns that track on influence dynamics will leverage future leap-ahead technologies in neural measurement, such as wireless EEG graphene tattoos that will enable non-intrusive measurement of social dynamics.

decision tasks, and hypothesized that lower spectral power in the alpha band is associated with certainty and higher spectral power is evident in uncertain decision situations, such as when expectations are violated. Using feedback-related negativity (FRN) event-related potential analyses, the team demonstrated that when expectations are violated, there is a significant difference in the amplitude of the lower band (Figure 1). This remarkable discovery represents a new way to detect neural signals of dominance contests. In 2020, the team published the results in *Social Psychology Quarterly* (Kalkhoff et al., 2020).

WAY AHEAD

These projects will become part of a workshop, along with other projects, showcasing the potential for using biophysiological measurement to track emergent social dynamics, including influence, power shifts, and emotion diffusion. The workshop will bring together researchers across the Army interested in these technologies to chart pathways for enhancing group performance and enable detection of influential adversarial groups and actors. Initial presentation of project results is occurring through the FY21 Life Sciences Branch Review seminar series.

This success was made possible by:

Dr. Lisa Troyer, Life Sciences Branch

Citations:

Dippong, J. *Sociological Science* **7**, 291-313 (2020).

Dippong, J. & Kalkhoff, W. *Advances in Group Processes Advances in Group Processes* **35**, 51-74 (2018).

SUCCESS STORY

Undetectable Vocal Spectrum Patterns Identify Emerging Influential Actors

This project analyzed a critical low-frequency component of the vocal spectrum that reflects influence dynamics, documenting for the first time how group members unconsciously differentiate their use of this component based on their status in a group. Analysis of these spectra shows that higher-status actors use this component more than lower-status actors; that as status-based hierarchies in groups become increasingly robust, group members will begin to rapidly differentiate the degree to which they dominate the low-frequency component; and that observers of interaction rate the influence of those occupying the lower-frequency spectrum as greater than that of those ceding use of this part of the vocal spectrum as group interaction proceeds.

CHALLENGE

Researchers have long studied the relationship between social status and social influence, but in many instances, status is unknown and influence is only known at the end of a phase of group interaction, such as when a decision is made or a course of action is pursued. Ideally, researchers want to predict the emergent hierarchy and likely influencers, but existing methods relying on self-reports and observer reports of whether a particular group member is likely to be influential hold a marginal predictive value with substantial error, making these methods undesirable in high-risk, high-impact settings frequently confronted by the Warfighter.

ACTION

Knowing who is likely to emerge as an influential group member is a critical piece of information that can improve group decision-making, enable identification of individuals who are driving the agendas of adversaries, and facilitate successful negotiations and determination of coordination action among groups with common interests and agendas. Because this is an emergent phenomenon, the ability to leverage knowledge about influential actors requires understanding the dynamics of how influence arises. Also, it is well established that intrusive methods to identify influential actors, such as asking individuals who is influencing the group as the interaction unfolds or after it has concluded, are disruptive and dysfunctional in real-world settings where the usefulness of such information is time-sensitive. In 2016, recognizing the importance of identifying influencers through non-intrusive methods to the Warfighter, Dr. Troyer began to seek researchers pursuing novel approaches to the study of status and influence dynamics. One early career scientist, Dr. Joseph Dippong (University of North Carolina at Charlotte), emerged with an ambitious research agenda in social influence. Dr. Troyer worked with Dr. Dippong to cultivate a successful initial Young Investigator Program (YIP; now Early Career Program [ECP]) proposal to computationally model status hierarchies. In ongoing work with Dr. Dippong, Dr. Troyer requested that he develop a second proposal that would integrate his computational models of status emergence with work he had conducted earlier detecting influencers by analyzing their vocal spectrum. In 2017, ARO awarded a grant to Dr. Dippong to pursue this work.

"[R]esearchers can employ vocal accommodation measures to ascertain the underlying status and dominance structure of groups of any size, in limited or open interaction, within any particular set of scope conditions, and in naturalistic or laboratory settings."

– Dr. Joseph Dippong, University of North Carolina at Charlotte

RESULT

Dr. Dippong developed an innovative experimental protocol to (1) test the relationship between vocal acoustic spectrum dominance and social influence, and (2) investigate whether evolving patterns in the vocal spectrum could be used as a signal to identify when dominant actors emerged and how other group members' vocal acoustic patterns shifted with the emergence of dominance. Drawing on his prior research on vocal acoustic patterns, Dr. Dippong recognized that the human voice crosses a wide range of frequencies that can be separated into discrete waveforms, much as a prism separates visible light wavelengths, using fast Fourier transform (FFT) methods. The prior research indicated that 500 Hz is a critical threshold, below which dominance dynamics can be detected. Higher-status and more-influential actors tend to dominate this range of the vocal spectrum, which sounds like a murmur through a wall—what is being said cannot be detected, only the rise and fall of pitch through the spectrum. Above this spectrum, content of speech is detectable. Dr. Dippong's work showed that not only do higher-status actors dominate this lower-frequency range, lower-status actors tend to show considerably more variability in the range (Dippong, 2020).

Drawing on other communications literature on nonverbal and paraverbal tendencies of members of groups, Dr. Dippong recognized that lower-status group members tend to "accommodate" these tendencies of higher-status group members such that, for example, they mimicked body language, posture, and speaking tempos of higher-status actors over time. He generated a risky hypothesis that lower-status actors would engage in a similar manner of vocal accommodation, attempting to match the rise and fall of frequencies of higher-status actors, while also ceding dominance of the lower voice spectrum to the higher-status actors. Pushing this line of scientific reasoning further, Dr. Dippong proposed that groups would adopt such vocal acoustic dynamics, even if their status assignments in a group were not based on any known ability and were completely arbitrary. His results confirmed both claims: members of groups unknowingly adjust their vocal frequencies in interaction to accommodate the perceived status of one another such that higher-status actors (who are more influential in group decision-making) exhibit stable domination of the lower voice frequencies, whereas lower-status actors exhibit higher voice frequencies, but with greater variability and adjustment toward the frequency range dominated by the higher-status actor. Furthermore, these (arbitrarily assigned) higher-status group members exercise greater influence in the group, and additionally, these dynamics are exacerbated when status differentiation is greater. That is, influence and domination of the lower vocal spectrum by higher-status group members is greater to the extent that status differences are greater, and vocal accommodation occurs more rapidly and synchronously with increased status differences. Finally, it is important to note that the frequency levels at which these status and influence dynamics occur are not consciously detectable or controllable by humans, making it an ideal way to unobtrusively identify influential actors in groups, as well as group conflict and coordination. Reports from this project were published in *Sociological Science* (Dippong, 2020) and *Advances in Group Processes* (Dippong and Kalkhoff, 2018).

WAY AHEAD

The next steps of this project include further experiments that track vocal patterns in initially undifferentiated groups that are convened without prior knowledge of one another, in an attempt to identify emergent influence dynamics from the point at which the groups are first formed. Also, research is needed to confirm that this dynamic, observed in groups comprising mostly English speakers, occurs in different language cultures. The work will also be included in a planned workshop that will feature other research on biophysiological signals of social dynamics of relevance to the Army, including work on the neural dynamics of influence and emotion measurement and contagion using infrared facial thermography. The work is also being shared with AFC's DoIS as it evolves.

ARL Competencies:

- Biological and Biotechnology Sciences
- Humans in Complex Systems

Results

- Published two research reports in peer-reviewed journals.
- Identified an unobtrusive method to detect status, influence, and conflict processes within groups as part of broader thrust in biophysiological signals of social dynamics.

Anticipated Impact

This work may equip Warfighters with unobtrusive new capabilities for rapid detection of influencers, as well as identification of intragroup conflict, with fragile hierarchies, advancing Soldier lethality advantages in Army Multi-Domain Operations. This impact, however, requires additional research to assess the cross-culture viability of this signal as well as test the limits of its ability to accurately detect emergent status and influence.

ATOMIC AND MOLECULAR PHYSICS PROGRAM

Program Manager
Dr. Paul M. Baker

Dr. Baker completed his undergraduate studies at Wright State University, receiving his B.S. in Physics in 2002. He trained as an atomic physicist at Tufts University, receiving his Ph.D. in Physics in 2009.

He came to ARO in 2010 as the Program Manager of the Atomic and Molecular Physics Program.

Current Scientific Objectives

1 | Drive investments in correlated quantum systems to enhance metrology (precision timekeeping) and reduce measurement uncertainty to the fundamental limit, while demonstrating insensitivity to noise from non-ideal environments (i.e., outside the laboratory) that, if successful, will provide assured navigation and global picosecond-level time synchronization.

2 | Discover, develop, and verify neutral atomic and molecular schemes for computational optimization, topological protected states (i.e., properties of a system that are global and related to the internal configuration), and emergence in complex systems that, if successful, will provide critical understanding of the mechanisms of novel materials that will enable the design of new material properties.

This success was made possible by:

Dr. Paul M. Baker, Physics Branch

Citations:

Norcia, M. A. *et al.* *Science* **366**, 93-97 (2019).

Young, A. W. *et al.* *Nature* **588**, 408–413 (2020).

SUCCESS STORY

Seconds-Scale Coherent Optical Clock

Professor Adam Kaufman's group at the University of Colorado developed new methods for simultaneously reaching large tweezer arrays (focused beams of light) of 320 sites for strontium atoms, while setting a new record for quantum coherence at optical frequencies. ARO made early investments to help pioneer this new method that makes progress toward DoD goals of picosecond-level, global-scale synchronization, assuring positioning, navigation, and timing (PNT) overmatch and robust networks.

CHALLENGE

The preparation and control of large arrays of qubits, the basic unit of quantum computation, are essential assets for computing, simulation, and metrology beyond the classical. Typically, control and scalability are at odds, as the more qubits one has, the harder it is to maintain and control quantum coherence simultaneously for all of the qubits. Optical tweezer arrays of neutral atoms have emerged as a promising route for threading this needle, allowing large arrays of individually trapped atoms that may be addressed and controlled. However, this technology is immature and the science is not well understood.

ACTION

Dr. Baker, the ARO Atomic and Molecular Physics Program Manager, monitored the impressive work of Professor Kaufman since he was a graduate student at the University of Colorado. His contributions to atomic physics, specifically his work on the atomic gas microscope experiment while a Postdoctoral Fellow at Harvard University, brought significant advances to the field. Dr. Baker approached Professor Kaufman once he had accepted his position as a full professor at the University of Colorado and discussed what scientific direction he would pursue. This discussion led to a Short-Term Innovative Research (STIR) award for the development of a tweezer array clock. Progress achieved on the high-risk STIR effort led to further investment via a Defense University Research Instrumentation Program (DURIP) award, which enabled investing in the key research components needed to rapidly accelerate the pioneering innovation of the Kaufman group. These early demonstrations and convincing vision resulted in a new four-year grant to develop a new method for entangled atomic clocks. The success of this approach is captured in recent *Science* and *Nature* publications (Norcia et al., 2019; Young et al., 2020) that report new records in atomic clock performance and establish the scientific basis for the DoD's vision to operationalize picosecond-level, global-scale synchronization.

RESULT

Professor Kaufman and his research team developed a method for creating tweezer array systems (highly focused lasers used to trap single atoms) that ultimately led to advancements in entangled atomic clock performance (Figure 1). This advancement was made possible by using two different tweezer wavelengths, 515 and 813 nm. The 515-nm tweezer array system is ideal for state preparation, ground-state cooling, and detection, while the 813-nm tweezer array system is ideal for constructing the axial lattice for clock spectroscopy. Because the 813-nm array is now only used for the clock lattice, it is used for shallow traps, where there is little power needed per atom. By realizing state-preserving transport between the arrays, the group could combine the strengths of both arrays individually and overcome previous challenges. This allowed the group to increase the atom number by a factor of 30 (i.e., trapped atoms in 320 different tweezers [160 atoms on any shot]).

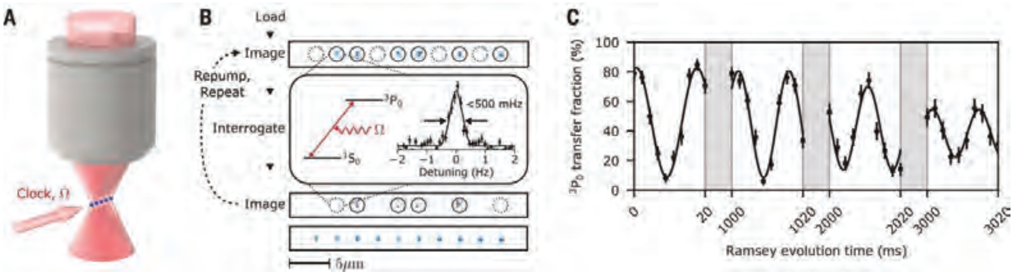

Figure 1: Clock transition interrogation in an optical tweezer array. (A) Apparatus for interrogation of $^1S_0$ to $^3P_0$ "clock" transition in tweezer arrays of strontium atoms. Using a high-numerical aperture (NA > 0.65) objective, the Kaufman group project tightly confining optical potentials to trap single strontium atoms. By tuning these traps near the so-called "magic" wavelength, they could ensure that the clock transition is minimally sensitive to the local intensity experienced by the atoms. (B) Repeated interrogation of clock transition. Top: Image of a single ensemble of atoms loaded into tweezers with ~50% filling. After interrogating the clock transition, excitation of the $^3P_0$ state can be inferred from apparent atom loss in a second image. By repumping atoms between interrogation cycles, each ensemble can be interrogated many times before losing atoms. Bottom: Image averaged over many such ensembles. Inset: Narrow-line Rabi spectrum of clock transition retrieved without repeated interrogation. Fits to sync and Gaussian functions are shown in gray and black, respectively. In this case, a 1.5-s probe yields an approximately Fourier-limited Gaussian linewidth of 450 ± 20 mHz. (C) Ramsey spectroscopy in 200-photon recoil energy (E_R) deep tweezers, showing a coherence time of 3.4 ± 0.4 s. The frequency of the fringes is set by the differential light shift imposed on the clock transition by the probe beam. These data were taken using the repeated imaging technique. Adapted from Norcia et al. (2019).

As mentioned, this new technique provided unanticipated gains for clock performance, as documented in high-profile publications in *Science* (Norcia et al., 2019) and *Nature* (Young et al., 2020). The large atom number and the single-site resolution allowed a number of novel and ground-breaking observations. Firstly, by having many atoms, the group could get single-shot measurements of the ensemble spin projection. As a result, they could see that the atomic coherence time was 20 s for an ensemble of 150 atoms.

By using correlation measurements through single-atom resolved imaging, the group were able to see that the single-atom coherence time was 48 s. These were coherence time records for both an ensemble and a single-particle optical clock transition. Correspondingly, this allowed the group to perform relative stability measurements, yielding an order-of-magnitude improvement in the measured stability from previous results. This most recent stability measurement was on par with present state-of-the-art measurements with optical lattice clocks.

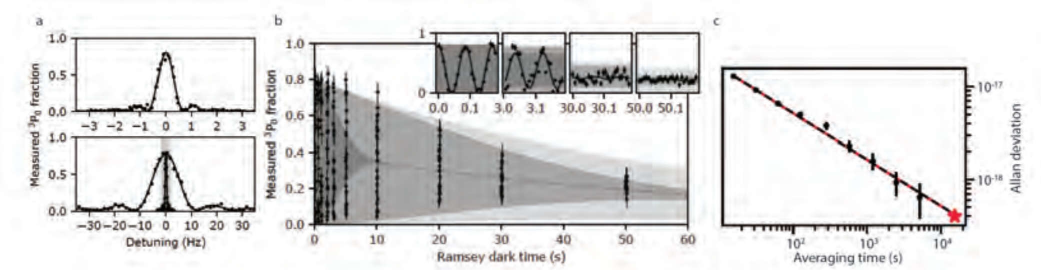

Figure 2: Scalable tweezer-array clock with half-minute atomic coherence and high stability. (A) Using the methods described, the Kaufman group created homogeneous arrays where the clock transition varied by much less than 50 mHz atom to atom; the data here is the averaged spectroscopic signal over the whole arrays. (B) Single-shot measurements of the atomic coherence, its variance, as well as correlation measurements (not shown) showing that the ensemble averaged atomic coherence lasts for ~ 20 s, while the single-atom coherence time lasts for 48 s. (C) Using the long coherence time and large atom number, demonstrate a stability of 5.2 × $10^{-17}(\tau/s)^{-1/2}$ and relative frequency precision between sub-ensembles of 4.2 × 10^{-19}. Adapted from Young et al. (2020).

ARL Competencies:

Sciences of Extreme Materials

Photonics, Electronics, and Quantum Sciences

Network Science and Computational Sciences

Results

- Led to an academic researcher from the Kaufman group applying to ARL to provide the Army with in-house expertise in this area.
- Developed quantum systems that work in non-ideal environments (i.e., outside the laboratory).

Anticipated Impact

Robust quantum metrology is expected to enable future leap-ahead technologies such as assured PNT and improved synchronized networks. The development of more accurate and more precise atomic clocks will enable the future U.S. Army to "own time," providing networks and computation systems unprecedented synchronization and computational capacity for operations within the enemy's decision space.

Specifically, using the methods described, the Kaufman group was able to create very homogeneous arrays where the clock transition varied by much less than 50 mHz atom to atom (Figure 2). The Kaufman group was able to see with single-shot measurements of the atomic coherence, its variance, as well as correlation measurements that the ensemble averaged atomic coherence lasts for approximately 20 s, while the single-atom coherence time lasts for 48 s. Using the long coherence time and large atom number, the Kaufman group demonstrated stability of $5.2 \times 10^{-17}(\tau/s)^{-1/2}$ and relative frequency precision between sub-ensembles of 4.2×10^{-19}.

WAY AHEAD

Overall, this work establishes several concepts and prospects: (1) it shows that the tweezer-array clock is a competitive technology for optical atomic clocks, (2) high precision accuracy studies are now possible given the high stability, and (3) the combination of individual atomic control and long coherence times on an optical clock transition establishes the near-term prospect of programmable entangled quantum sensors and establishes the scientific basis for the DoD's vision for picosecond-level, global-scale synchronization. The Kaufman group is now pursuing new Rydberg dressing approach below that, if successful, could provide additional stability and performance.

This success was made possible by:

Dr. Paul M. Baker, Physics Branch

Citations:

Borish, V., Marković, O., Hines, J. A., Rajagopal, S. V. & Schleier-Smith, M. *Phys. Rev. Lett.* **124**, 063601 (2020).

SUCCESS STORY

Transverse-Field Ising Dynamics in a Rydberg-Dressed Atomic Gas

Professor Monika Schleier-Smith's group at Stanford University demonstrated long-range Ising interactions in a cold gas of cesium atoms using the Rydberg dressing method. The group characterized the Ising interactions by measuring the mean-field shift of the clock transition via Ramsey spectroscopy, observing one-axis twisting dynamics. In addition, the group was able to emulate a transverse-field Ising model by periodic application of a microwave field and detect dynamical signatures of the paramagnetic–ferromagnetic phase transition. This result highlights the power of optical addressing for achieving local and dynamical control of interactions, enabling prospects ranging from investigating Floquet quantum criticality to producing tunable-range spin squeezing.

CHALLENGE

Optically controlled interactions among cold atoms are a powerful tool for fundamental studies of quantum dynamics and engineering entangled states. Theoretically, tailoring interactions with light allow for accessing nonequilibrium phases of matter, studying inhomogeneous quantum phase transitions, implementing quantum optimization algorithms, and enhancing quantum sensors.

An alternative to direct excitation is the method of Rydberg dressing (i.e., inducing interactions among ground-state atoms by coupling to Rydberg states with an off-resonant laser field). Rydberg dressing offers the benefit of dynamical control over the strength and form of interactions, as well as a long coherence time once the light is switched off. Maximizing the coherence of the interactions themselves has been the focus of several recent experiments. While dressing in dense 3D lattices has suffered from runaway loss and dephasing, Rydberg dressing has been successfully applied to electrometry in a bulk gas, entangling atoms in optical tweezers and studying coherent many-body spin dynamics in 1D and 2D atom arrays.

The key to realizing both of these objectives is the ability to trap and image single atoms, so as to venture beyond mean-field dynamics into the deeply quantum regime. To this end, Professor Schleier-Smith and her research group recently began trapping atoms in optical tweezers and observed the first single-atom signals, and are currently optimizing the loading and imaging of a tweezer array.

ACTION

A major accomplishment of Professor Schleier-Smith's group was the realization of a Floquet transverse-field Ising model in a Rydberg-dressed atomic gas. By probing the mean-field dynamics of this model, the Schleier-Smith group observed signatures of a paramagnetic-to-ferromagnetic phase transition. Extensions to this work will enable (1) investigating frustrated antiferromagnetic Ising models and (2) exploring a rich diagram of Floquet phases including ones with no equilibrium analog, such as the Floquet symmetry-protected topological (SPT) phase.

These results highlight capabilities for local and dynamical control of interactions that make Rydberg dressing an exceptionally versatile tool for quantum simulation. Previous work by Professor Schleier-Smith's research team was focused on a regime that rapidly alternated between Ising interactions and a transverse field to mimic a static transverse-field Ising model. Varying the drive period will then allow

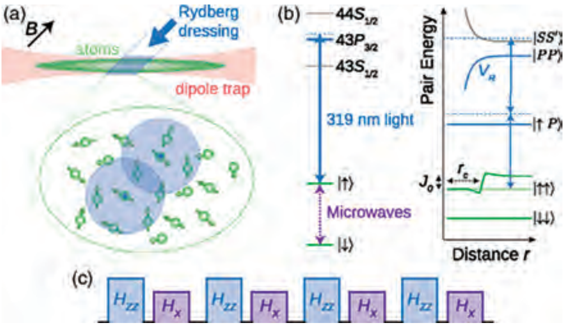

Figure 3: Experimental setup and Rydberg dressing scheme. (A) A cloud of cesium atoms is held in an optical dipole trap and locally illuminated with 319-nm light to generate Ising interactions of characteristic range r_c and strength J_0. The quantization axis is set by a 1-G magnetic field. (B) Energy-level diagrams for a single atom (left) and a pair of atoms (right). (C) Alternating between interactions (H_{zz}) and microwave rotations (H_x) produces an effective transverse-field Ising model. Adapted from Borish et al. (2020).

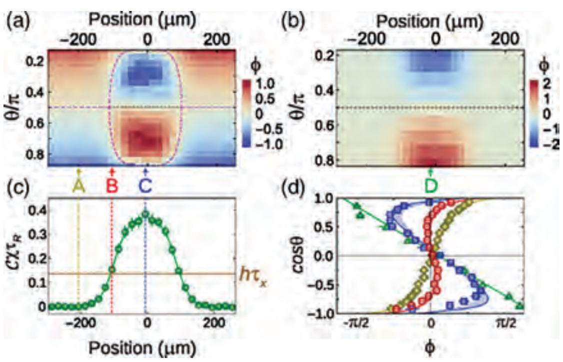

Figure 4: Dynamical signature of paramagnetic-to-ferromagnetic phase transition. (A,B) Phase φ of the average Bloch vector after the Floquet sequence of Figure 3, as a function of initial tilt θ of the Bloch vector and position in the atomic cloud, for (A) Ising interactions with transverse field or (B) Ising interactions only. The φ = 0 contour reveals fixed points of the mean-field dynamics, showing a bifurcation at the paramagnetic-to-ferromagnetic phase transition. Fitting the phase evolution in (B) yields the average mean-field interaction per cycle, shown in (C) by green points and the fit curve. (D) Final phase φ vs. initial tilt θ for cuts labeled A (yellow diamonds), B (red circles), C (blue squares), and D (green triangles), in order of increasing interaction strength. Adapted from Borish et al. (2020).

for accessing the predicted Floquet SPT phase. The Schleier-Smith group has already demonstrated the ability to realize either sign of interaction (ferromagnetic or antiferromagnetic) by choice of Rydberg state and laser detuning, which paved the way to investigating frustrated antiferromagnetic models. The ground states of these frustrated Ising models can be found by implementing a quantum approximate optimization algorithm (QAOA), which applies Ising interactions and a transverse field in an alternating sequence (Figure 3).

In addition to the experimental progress, the Schleier-Smith group showed that Rydberg dressing offers a promising route to solving the combinatorial optimization problem of number partitioning by enabling a hardware-efficient implementation of Grover's search algorithm. This problem exhibits a phase transition in computational complexity that makes it an ideal case study for elucidating the physical manifestations of computational complexity (Figure 4). The Schleier-Smith group's theoretical work includes a detailed analysis of the performance attainable in realistic near-term experiments, showing prospects for attaining a quantum speedup for small systems even in the hard phase.

RESULT

This work opens prospects in quantum simulation benefiting from spatiotemporal control of interactions, including exploring quantum criticality in both driven and spatially inhomogeneous systems. The ability to emulate a static transverse-field Ising model, varying the strength of interaction and/or rotation per Floquet cycle, will allow for accessing quantum phases with no equilibrium analog, including Floquet symmetry-protected topological phases.

Combining Floquet driving with a spatially varying interaction strength may allow for realizing quantum systems with emergent spacetime curvature. The Ising interactions demonstrated can also be applied to generate entangled states for enhanced clocks or sensors, with dynamical control of interactions and the transverse field enabling enhanced spin squeezing. Spatial addressing will additionally allow for preparing arrays of entangled states for optimal atomic clocks, such as the work presented in the previous Success Story Professor Kaufman's group.

WAY AHEAD

By developing this method of Rydberg dressing the Schleier-Smith group has provided a new experimental platform for studying fundamental quantum interactions with spatial control in quantum many-body systems. This is important for understanding and discovering new material properties. Due to the complexity of the systems being investigated, theory is computationally challenging, so this experimental access is vital. In addition, this new method has already been shown to improve clock performance as indicated by the previous work by the Kaufman group. Future work seeks to demonstrate a quantum speedup over classical computers in hard phases, which would provide important insights into the limits of computation. This project's success demonstrates how the Atomic and Molecular Physics Program funding strategy can impact outcomes across a variety of efforts by making investments in fundamental research.

ARL Competencies:

- Sciences of Extreme Materials
- Photonics, Electronics, and Quantum Sciences
- Network Science and Computational Sciences

Results

- Made discoveries that improve the performance of quantum systems and ensure quantum systems perform in non-ideal environments.
- Advanced ARL SEDD Rydberg dressing and quantum information science (QIS) research.

Anticipated Impact

The methods being developed will lead to improvement in atomic clocks and quantum sensors. In addition, these methods can be applied to quantum simulation for new materials as well as quantum computation by leveraging Grover's algorithm. The development of more accurate and more precise atomic clocks will enable the future U.S. Army to "own time," providing networks and computation systems unprecedented synchronization and computational capacity for operations.

QUANTUM INFORMATION SCIENCE PROGRAM

Program Manager
Dr. Sara Gamble

Dr. Gamble completed her undergraduate studies at the University of Florida, receiving her B.S. in Physics in 2003. She continued her education at Stanford University, receiving her Ph.D. in Applied Physics in 2010.

She came to ARO in 2017 as the Program Manager for the Quantum Information Science Program.

Current Scientific Objectives

1 | Extend our understanding of multi-qubit and entangled quantum systems to ultimately enable advances in quantum computation and quantum networks that, if successful, could enable beyond classical capabilities in computation, communication, and sensing.

2 | Establish the limits of the advantages of qubit-based quantum systems over classical systems for sensing and measurement that, if successful, could enable sensitivities physically unachievable by traditional, classical systems.

3 | Devise novel, primarily non-cryptographic-focused algorithms to expand the application space of quantum information processing that, if successful, could enable breakthroughs in fields ranging from machine learning, to optimization, to chemistry and materials science.

This success was made possible by:

Dr. Sara Gamble, Physics Branch

Dr. T. R. Govindan, NASA; Physics Branch

Dr. Samuel Stanton, Mechanical Sciences Branch

Citations:

Majumder, S., de Castro, L. A. & Brown, K. R. *npj Quantum Inf.* **6**, 19 (2020).

SUCCESS STORY

Integrated Quantum Sensing and Control for High-Fidelity Qubit Operations

Army researchers developed the theoretical foundations for a novel calibration approach for quantum information science experiments. If implemented successfully, the scheme will enable longer, more complex qubit-based experiments that are crucial to reach the Army goal of leveraging the quantum properties of matter for beyond classical capabilities in information gathering, processing, and sharing for overmatch.

CHALLENGE

Realizing the full capabilities of quantum information processing systems will require the ability to carry out operations on qubits with very low error rates, even in the presence of noise and others sources of decoherence. Achieving these low rates is, however, notoriously difficult. A primary challenge is that scientists often lack a full picture of the character of the noise and, without a full characterization, control and mitigation strategies are difficult to devise. An additional challenge is implementing any devised control and mitigation strategies effectively on the timescales required for many quantum experiments and implementations.

ACTION

Since its inception, quantum information science has been a multidisciplinary endeavor. A merging of information science and quantum physics created it, but as the field matured and grew, so did the breadth of disciplines needed to sustain it. Over the past several years, a multidisciplinary focus on qubit physics, materials, fabrication, and operation became crucial in the effort to successfully create and manipulate qubits, the fundamental unit of quantum information.

Qubits and their associated quantum states are often fragile entities. Noise from factors such as uncontrolled magnetic, optical, or microwave fields; bias voltages and currents; temperature; and pressure can all destroy the quantum states necessary for quantum information science applications.

Thus, control techniques that can mitigate common noise sources are key for nearly all quantum information experiments. In parallel with advances related to the qubits themselves, computer science, statistics, and engineering-based control techniques were employed by quantum scientists in the field to develop novel quantum control and feedback approaches.

During the FY18 Multidisciplinary University Research Initiative (MURI) topic development cycle, Dr. Gamble began to think more closely about these control approaches. In state-of-the-art experiments, the classical environment in which the qubits sit was rarely fully characterized. Logically following, if one does not have a full picture of the environment and all the sources of noise, one cannot correct for them.

At this point Dr. Gamble and Dr. T. R. Govindan, Program Manager for the Fault-Tolerant Quantum Computation external program, began discussing these issues of characterization and control. They had a key insight: to increase our control over noise, we need to have better sensors to characterize that noise. Empirically, this sensing in quantum information experiments had been done with classical sensors—like magnetometers and thermometers common across disciplines. A large component of Dr. Gamble's investments in quantum information science, however, are devoted to a different kind of sensing: qubit-based quantum sensing. Qubits often provide the most sensitive and precise measurements of the variability and noise in the classical environment in which they operate and, consequently, serve as high-performance sensing and metrology tools. Why then, are quantum sensing and quantum computing experiments often distinct from one another? Why not bring the exquisite sensitivity of quantum sensors into quantum computation platforms for enhanced characterization, hopefully leading to enhanced control?

Drs. Gamble and Govindan began working with the Complex Dynamics and Systems Program Manager and expert in classical control, Dr. Samuel Stanton, to craft a MURI topic with the goal of setting a new paradigm for the field—real-time control of the qubit classical environment via a novel combination of qubit sensing, statistics, machine learning, and control approaches. In this new paradigm, qubit sensor-based characterization and verification of classical environmental fields are conducted by a distinct set of "spectator" qubits located in the vicinity of the data qubits carrying out quantum operations. In this scheme, directly proposed by the program managers in the topic and a departure from typical MURI topic formulation, spectator qubit measurements are inputs in advanced dynamic "closed" loop feedback control strategies that result in fully characterized, verified, and controlled classical environment fields, thereby enabling the realization of very high-fidelity data qubit operations.

A team lead by Professor Kenneth Brown at Duke University was selected to pursue this novel concept. Additionally, the innovative scheme drew the attention of the Australian government and, with their support, three Australian partner universities joined the research effort. This partnership made this MURI not only a true multidisciplinary effort, but a multinational one as well.

To further this international partnership, Dr. Gamble, Dr. Govindan, and Professor Brown decided to hold the first year review of the MURI in Sydney, Australia, in October 2019. Scientific program managers from the United States joined Drs. Gamble and Govindan at the review, along with members of the Australian government involved in the work. Thus, the MURI became a platform to further enhance the strong relationship the United States and Australia have had for many years in quantum information science.

RESULT

While some sources of error can be mitigated or eliminated with a variety of techniques, it is significantly more difficult to correct errors that vary as a function of time and/or space. Not to shy away from a challenge, the MURI team decided to approach the theory behind how to tackle these errors with the spectator qubit concept early on.

Approaches to handle these varying errors often cannot achieve the desired error reductions because of the relatively long amount of time it takes to extract information about the error parameters from the system. To achieve the necessary level of control to ensure successful quantum operations, the team made the key insight

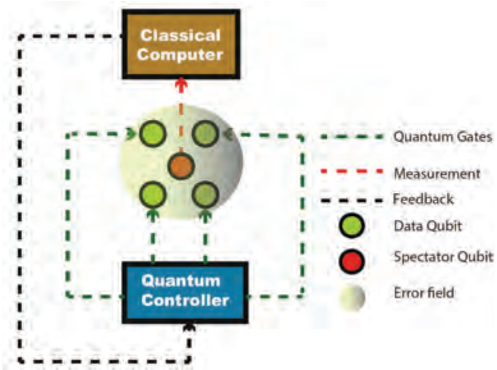

Figure 1: General feedback loop for spectator qubits. Information about errors is acquired by the spectator qubits. This information is subsequently analyzed by a classical apparatus that then updates the optimal control strategy for the data qubits to increase the time the data qubits can be used for quantum information processing. Figure and caption adapted from Majumder et al. (2020).

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Network Science and Computational Sciences

Results

- Established the theoretical foundations for a novel calibration approach for quantum information science experiments.
- Enhanced international partnership between the United States and Australia in the quantum sciences.
- Co-published a paper between U.S. and Australian scientists (Majumder et al., 2020).

Anticipated Impact

Going forward, it is anticipated that spectator qubit schemes like the one developed by the Duke team will enable error rates below the threshold for fault-tolerant operation for times longer than otherwise possible. Achieving fault-tolerant operation of qubit systems would be a milestone for the field and is a crucial step in elucidating how to create and control the large-scale qubit-based systems the Army needs for quantum computation and distributed quantum information applications such as networking.

that the acquisition of information from the spectator qubits has to be faster than the rate at which errors accumulate on the data qubits. By using control strategies that minimize the sensitivity of the data qubits involved in computations, the system can acquire sufficient information from the spectator qubits to update the estimates of many error parameters and improve overall control (Figure 1).

As a result, the approach can increase the length of time that data qubits function reliably to ultimately enable more complex quantum computations. The team simulated how the use of spectator qubits in their proposed control schemes can keep data qubit error levels below a threshold of 10^{-4} in two situations of high experimental relevance: magnetic-field noise and laser beam instabilities.

WAY AHEAD

The MURI team will continue to develop novel methods for spectator qubit-based characterization and expand the application space of this approach. While this work is looking toward future quantum computing systems, in the near term, the success of the described approach could likely be enhanced if small corrections in the calibrations could be made after fewer spectator measurements.

This success was made possible by:

Dr. Sara Gamble, Physics Branch

Dr. T. R. Govindan, NASA; Physics Branch

Citations:

Cao, Y. *et al. Chem. Rev.* **119**, 10856–10915 (2019).

SUCCESS STORY

From Quantum Algorithms to Quantum Startups to Quantum Partnerships

Novel quantum algorithm work originally supported by ARO for potential quantum chemistry applications led to the founding of a startup company now partnering with ARL scientists to explore the application of small quantum computers to Army-relevant problems.

CHALLENGE

Elucidating the types of problems that future quantum computers will be able to solve more efficiently than any classical computer is incredibly difficult. While researchers know some types of applicable problems, such as the factoring of large numbers into their primes, are amenable to incredible speedup on a quantum computer, scientists do not have a general formula or prescription for which types of problems will or will not be amenable to these speedups. While quantum algorithms that simulate quantum chemistry on a quantum computer are likely able to obtain results that are intractable classically, it is not well understood how to do this with low overhead, such as with a minimum number of quantum computations, and high accuracy.

ACTION

In the study of quantum algorithms, the ultimate goal is always to obtain a quantum algorithm that solves a problem which a classical algorithm cannot. Here, “cannot” means cannot solve in any time of practical relevance, like the lifetime of the universe. Quantum chemistry was one of the first disciplines envisioned to be amenable to a quantum speedup, an idea largely pioneered by Richard Feynman in the 1980s. Envisioning a result and producing the concrete approach to achieve it, however, are quite different.

When Dr. T. R. Govindan had the role of Quantum Information Science Program Manager prior to Dr. Gamble joining ARO, he began supporting work by Professor Alán Aspuru-Guzik from Harvard University. The work aimed to understand how quantum chemistry can be simulated on a quantum computer with the most efficient overhead and accuracy (Figure 2). It drove toward an understanding of the lowest-possible overall scaling of the quantum algorithms as a function of molecular size and the lowest-possible quantum gate count. Here, “gate count” is essentially one measure of how difficult an algorithm would be to run on a quantum computer. By the time Dr. Gamble joined ARO, developing these understandings was of growing importance to not only burgeoning DoD programs, but to the quantum computing community as a whole.

While one of the long-term visions for quantum computation is to carry out fault-tolerant, error-corrected computations on complex systems comprising multiple qubits, that goal is many years, and likely many decades, away. In the meantime, the question of whether we can use near-term noisy intermediate-scale quantum (NISQ) devices for any practical advantages for some set(s) of problems has become prominent.

One leading candidate type of algorithm that may exhibit some type of quantum advantage on these NISQ systems is the Variational Quantum Eigensolver (VQE). This type of algorithm was one under study in Professor Aspuru-Guzik’s ARO work. While traditional quantum algorithms with guaranteed

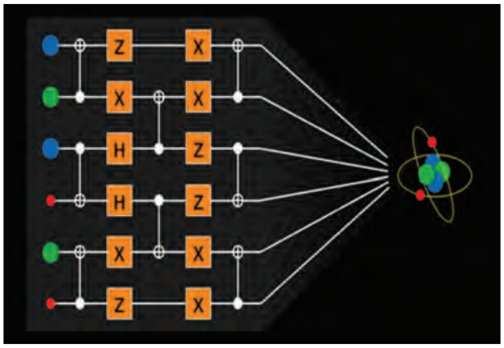

Figure 2: Quantum computers and quantum chemistry. Since quantum computers inherently use the properties of quantum mechanics to operate, they are naturally suited to try to tackle inherently quantum mechanical problems like those of quantum chemistry. Quantum chemistry problems are a class of problems that may be amenable to running on noisy, near-term quantum computers. Figure and caption adapted from Cao et al. (2019).

performance generally require the fault-tolerant operations described previously, VQE algorithms seek to remove this requirement by reformulating the computation. This allows for an expansion of operability in devices that lack error correction, such as NISQ devices.

The convergence of the availability of NSIQ devices from large and small companies, the technology and founders of which were almost all supported in their academic work by ARO in some capacity, and the insights into the quantum algorithms that may be amenable to showing quantum advantages on them led to Professor Aspuru-Guzik leveraging his ARO-supported work to found a startup company, Zapata Computing Inc. (Zapata).

While Professor Aspuru-Guzik set the foundations for his company, he continued to work with ARO support on foundational, basic research questions of interest to the Army. In mid-2018, however, a new opportunity emerged. With Zapata at that point relatively established as a startup on the foundations of ARO-supported work, could the Army learn anything by directly partnering with the company in addition to partnering in the basic research space?

The new ARO Program Manager Dr. Gamble, now managing Professor Aspuru-Guzik's grant, and ARL Northeast initiated conversations to delve into this question. Dr. Gamble was the only Army representative in these conversations with a background in quantum sciences and was thus crucial in the process of deciding if the Army should initiate partnership conversations with Zapata, a question that, thanks to her subject-matter expertise, was ultimately decided in the affirmative.

Partnership conversations with Zapata immediately involved scientists who were previously directly supported by ARO quantum algorithm grants. That support was not limited to students or post-docs supported through the Professor Aspuru-Guzik's grant, but other grants as well. This serves as a testament to not only the high caliber of researchers ARO generates, but also the cohesiveness of the programmatic goals—here to work toward the understanding and establishment of quantum algorithms that provide a quantum advantage. These scientists worked together informally as participants in ARO grants and are now working formally together toward the common goal of demonstrating quantum advantage for real-world problems.

RESULT

Two central questions of interest emerged from initial face-to-face meetings between the Zapata Computing and ARL teams: (1) can we learn about the effectiveness and limitations of Zapata's algorithmic approach by applying it to real Army problems and (2) can we potentially establish an advantage for problems of high Army relevance when computed on the NSIQ devices Zapata works with versus the best-known classical alternative?

These questions were deemed of high enough academic and technical merit to establish a cooperative research and development agreement (CRADA) between the Adelphi Laboratory Center (ALC) and Zapata Computing to explore them. ARO Program Manager Dr. Gamble was instrumental in laying the ground work for this agreement with respect to establishing trust with the Zapata team and setting the expectations of what we may, or may not, learn from the work.

Currently, ARL scientists are working with Zapata to define the first problems to consider as a team. A benchmarking study will likely be the first, to establish that the quantum approaches obtain the same answer to problems ARL already knows how to solve. Looking forward, problems that are more complex will be under consideration in FY21.

WAY AHEAD

This is an effort through which ARL may be a true first adopter of entangled quantum technology to solve Army-relevant problems in the mechanical sciences.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Network Science and Computational Sciences

Results

- Supported ARO foundational research in quantum chemistry algorithm development that was then leveraged by the principal investigator in the establishment of his startup company, Zapata Computing Inc.
- Allowed the Army, via a newly established FY20 CRADA between ALC and Zapata, to be a first potential adopter to use quantum computers in Army-relevant problems in the mechanical sciences.

Anticipated Impact

ARO is continuing to identify and support efforts to drive the advancement of both the fundamentals of quantum algorithms and the qubit-based science needed to execute them. This combination will likely lead to overmatch capabilities in information processing in the decades to come.

ARO IN THE NEWS

New research advances Army's quest for quantum Networking

BY U.S. ARMY DEVCOM ARMY RESEARCH LABORATORY PUBLIC AFFAIRS | JUNE 24, 2020

Two U.S. Army research projects advance quantum networking, which will likely play a key role in future battlefield operations.

Quantum networks will potentially deliver multiple novel capabilities not achievable with classical networks, one of which is secure quantum communication. In quantum communication protocols, information is typically sent through entangled photon particles. It is nearly impossible to eavesdrop on quantum communication, and those who try leave evidence of their tampering; however, sending quantum information via photons over traditional channels, such as fiber-optic lines, is difficult – the photons carrying the information are often corrupted or lost, making the signals weak or incoherent.

In the first project, the University of Chicago research team, funded and managed by the U.S. Army's Combat Capability Development Command Army Research Laboratory's Center for Distributed Quantum Information, demonstrated a new quantum communication technique that bypasses those traditional channels. The research linked two communication nodes with a channel and sent information quantum-mechanically between the nodes—without ever occupying the linking channel.

> **"This result is particularly exciting not only because of the high transfer efficiency the team achieved, but also because the system they developed will enable further exploration of quantum protocols in the presence of variable signal loss," said Dr. Sara Gamble, program manager at the lab's Army Research Office and co-manager of the Center for Distributed Quantum Information. "Overcoming loss is a key obstacle in realizing robust quantum communication and quantum networks."**

The research, published in the journal Physical Review Letters, developed a system that entangled two communication nodes using microwave photons—the same photons used in cell phones—through a microwave cable. For this experiment, they used a microwave cable about a meter in length. By turning the system on and off in a controlled manner, they were able to quantum-entangle the two nodes and send information between them—without ever having to send photons through the cable.

> **"We transferred information over a one-meter cable without sending any photons to do this, a pretty unusual achievement," said Dr. Andrew Cleland, the John A. MacLean Sr. Professor of Molecular Engineering at Pritzker Molecular Engineering at University of Chicago and a senior scientist at Argonne National Laboratory. "In principle, this would also work over a much longer distance. It would be much faster and more efficient than systems that send photons through fiber-optic channels."**

Though the system has limitations, it must be kept very cold, at temperatures a few degrees above absolute zero, the researchers said it could also potentially work at room temperature with atoms instead of photons.

The team is now conducting experiments that would entangle several photons together in a more complicated state, which could ultimately enable enhanced quantum communication protocols and capabilities.

Entangled particles aren't just limited to photons or atoms, however. In a second paper published June 12 in the peer-reviewed journal *Physical Review X*, the same Chicago team entangled two phonons—the quantum particle of sound—for the first time.

Using a system built to communicate with phonons, similar to the photon quantum communication system, the team entangled two microwave phonons, which have roughly a million times higher pitch than can be heard with the human ear.

Once the phonons were entangled, the team used one of the phonons as a herald, which was used to affect how their quantum system used the other phonon. The herald allowed the team to perform a so-called quantum eraser experiment, in which information is erased from a measurement, even after the measurement has been completed.

> **"Phonons give you a much bigger time window to do things and relieve some of the challenges in doing a quantum eraser experiment," Cleland said.**

Though phonons have a lot of disadvantages over photons—for example, they tend to be shorter-lived—they interact strongly with a number of solid-state quantum systems that may not interact strongly with photons. As a result, phonons could provide a better way to couple to these systems.

This coupling is a critical capability for many quantum networking applications, and may also benefit other quantum information science applications such as quantum computing. Additionally, the wavelengths of phonons are shorter than those of photons for the same frequency, potentially enabling smaller quantum circuits.

> **"Together, these experiments provide multiple avenues for future research into how we construct quantum networks that function in non-ideal environments, and reliably transfer quantum information between systems," said Dr. Fatemi, researcher at the laboratory and co-manager of the Center for Distributed Quantum Information. "Both are critically important for developing future quantum technologies."**

Senior Research Scientist Spotlight | Dr. Peter J. Reynolds
Senior Research Scientist, Physical Sciences, ARO

Dr. Reynolds has been a Senior Research Scientist at ARO since 2007. He is best known for his research in statistical mechanics, creating renormalization group methods for geometrical phase transitions, developing quantum Monte Carlo methods for solving the Schrödinger equation, and supporting foundational research leading to the emergence of quantum information science. He started at ARO as a Program Manager in Atomic and Molecular Physics and became Physics Branch (formerly Division) Chief in 2004.

Prior to joining ARO, Dr. Reynolds was a Program Officer at the Office of Naval Research from 1988-2003, a Staff Scientist at Lawrence Berkeley Lab from 1980-1988, and an Assistant Research Professor at Boston University from 1979-1980. He received the U.S. Presidential Rank Award as a Distinguished Senior Scientist in 2015 and is a Fellow of the American Physical Society.

Dr. Reynolds obtained his Ph.D. in Theoretical Physics from the Massachusetts Institute of Technology in 1979 and has an A.B. in Physics from the University of California, Berkeley.

Quantum networks are one part of the growing and evolving discipline of quantum information science (QIS). QIS has its roots in a talk that Richard Feynman gave circa 1980 where he asked the following: "Can a classical, universal computer simulate any physical system? And in particular, what about quantum systems?"

Because the state space that quantum systems live in (which is a Hilbert space) is exponentially higher in dimension than classical geometrical spaces in which ordinary mechanics "happens," quantum mechanical problems typically scale exponentially, making them effectively uncomputable for any but the smallest systems. Feynman suggested that to efficiently solve a quantum problem, one must therefore map the problem onto a quantum system. This is literally done nowadays and is called "quantum simulation." But back in ~1980, this was just an idea. This line of thought led people to wonder, "If quantum mechanics can exponentially speed up simulations, could such improvements exist elsewhere as well, not just with simulation?" For example, was it possible to exponentially speed up a computation by exploiting the laws of quantum mechanics? Such "quantum computing" was discussed in various (mostly physics) circles during that period for about a decade, but was largely a curiosity.

In 1994 Peter Shor, then at Bell Labs, made a major breakthrough that made quantum computing suddenly seem like something reasonable. He published a paper that gave an explicit algorithm for a quantum computer (were one to exist) to find the prime factors of a large number—the difficulty of which is the basis for the RSA cryptosystem and related public key encryption on which we all depend for secure transactions on the Internet—in polynomial time. In other words, he found an exponential speed-up for an algorithm (an algorithm of some significance) on a quantum computer!

It didn't take long for people to look at where else quantum physics might provide an edge over classical approaches. What emerged were areas such as quantum encryption (possibly to counter the loss of RSA-type encryption due to quantum computing), quantum communication more broadly, quantum sensing, quantum imaging, and the subject of this accompanying press release, quantum networking. In sum, these, together with quantum computing and quantum simulation, became the broader field of QIS.

In each of the above cases, it is important to note that the modifier "quantum" doesn't mean "better," though this is a common perception; a more apt word would be "different." To illustrate this, despite the advantages a quantum computer would have for breaking RSA encryption, it would not be an efficient way to do the majority of the kinds of computations that ordinary computers do. Most algorithms cannot be sped up this way, though there are a few interesting ones that can be, and it remains an active area of research to discover new ones. Thus, quantum computing is very much "special purpose" computing. Similarly, a quantum network will in no way be a replacement for ordinary networks (communications, computing, or otherwise). Instead, a quantum network would provide new functionalities.

This ability to control the individual atoms, actually further than Feynman was imagining, down to their very quantum states, was the experimental tool that was the enabler for implementing QIS. Up to this point in the discussion, all the QIS advantages were theoretical analyses.

Around this same time, when these quantum-enabled ideas were blooming (mid-1990s), this field that Feynman had in a way foreseen in the 1980s collided with another field that Feynman had similarly predicted—even earlier! In a lecture Feynman gave at the annual American Physical Society meeting at the California Institute of Technology on December 29, 1959, he considered the possibility of direct manipulation of individual atoms to build things from the ground up (e.g., for synthetic chemistry or creation and/or manipulation of materials). Very well known as the "There's Plenty of Room at the Bottom" talk, this led to what is now known as nanoscience. This ability to control the individual atoms, actually further than Feynman was imagining, down to their very quantum states, was the experimental tool that was the enabler for implementing QIS. Up to this point in the discussion, all the QIS advantages were theoretical analyses.

With this enabler, experimentation caught up quickly. Shor's algorithm had received immediate attention in the atomic physics community and was discussed at a 1994 international meeting of the community just a few months after Shor distributed a preprint of his work. Two atomic theorists present at the meeting, Ignacio Cirac and Peter Zoller, formulated an experimental way to create qubits, the fundamental elements (like bits for an ordinary computer) that would be needed in a quantum computer. Guided by Cirac and Zoller's paper, David Wineland, through DoD support by Dr. Reynolds, demonstrated the first qubit—in an ion trap. Though a direct result of Shor's work, via Cirac and Zoller's proposal, this work ended up being submitted at almost the same time that Shor's paper actually appeared in print, in the summer of 1995. QIS as a field was now born.

This same 1994 international meeting had two DoD program managers in attendance, one being Dr. Reynolds. Recognizing the importance of this new field the Army immediately organized a workshop to explore the various advantages quantum computing and quantum cryptography could provide. It was clear that even though Shor's algorithm was profound, solving exponentially "hard" quantum mechanics problems was going to directly impact the design of new materials, chemicals, and more, and that much more than this was possible.

The result of the Army workshop was one of those rare instances where a new dedicated ARO program was created. Quantum Computing joined Condensed Matter Physics, Atomic, and Molecular Physics and Optics and Imaging as a separate program in the ARO Physics Branch shortly thereafter.

Over the years, the investments made by ARO, and subsequently other funders, created a diverse ecosystem in QIS, spanning numerous sub-disciplines of physics, and beyond to mathematics, computer science, and materials science. More recently, engineering has been brought into the fold to form a broad and separate discipline called quantum information science and technology (QIST). This quantum information ecosystem is founded on the more exotic parts of quantum mechanics, particularly superposition and entanglement. While the majority of 20th-century physics was based on quantum mechanics and underlay advances ranging from the laser, to the transistor, to quantum chemistry—topics now dubbed as "quantum 1.0" —the exotic aspects, and entanglement in particular, were the enablers of "quantum 2.0." Quantum networking is in many ways the most nascent member of the family of quantum 2.0 disciplines.

After more than two decades of DoD investment and ensuing growth of this field, Dr. Reynolds, with support from ARO leadership, engaged with the office of the Assistant Secretary of the Army for Acquisition, Logistics, and Technology (ASA[ALT]) to formulate a Program Objective Memorandum (POM) 2015 investment recommendation that funds be allocated for ARL to invest in and pursue QIS in a serious way. For a decade, ARL had only had a single researcher doing work underpinning QIS, namely, attempting to create a Bose–Einstein condensate. In 2015, with the POM start, the question became what area within QIS to carve out for ARL.

It is difficult to argue that networks and communication are not major areas of Army relevance; they were areas that ARL was already heavily invested in (classically). Thus, it was decided by the leadership that the focus of ARL's QIS efforts would be in quantum networks. ARL hired a number of outstanding researchers for working in-house, in SEDD and CISD, and in parallel funded an extramural center (the Center for Distributed Quantum Information [CDQI]), all focused on the big, long-term scientific questions of creating quantum networks. This press release demonstrates progress in this work.

As mentioned, a quantum network is not a replacement for a classical network. But what is it? At its most fundamental, a quantum network distributes entanglement, which can be thought of as a quantum "resource," and maintains quantum coherence across network nodes. In fact, coherent superposition of states and entanglement lie at the heart of the power behind quantum information; they are the enabler of the exponential speed-up of Shor's algorithm and lie behind many other applications of QIS.

While superposition was well known in quantum mechanics, namely, that any quantum state could consist of sums of other quantum states, entanglement was even weirder. Though superposition states were involved in everyday 20th-century quantum mechanics, they nevertheless presented paradoxical thought experiments, such as Schrödinger's cat: in principle, a cat could be simultaneously both alive and dead. But Einstein found entanglement even weirder and rejected it as "spooky action at a distance." In fact, this is what makes it so powerful. At its core, entanglement is a correlation between separated objects that is greater than is classically possible. What made it spooky to Einstein was that the correlations were instantaneous, with a measurement on one object immediately determining aspects of the state of the other. This seemed to violate causality, a foundation of Einstein's theory of relativity. It was only much later that it was proven that despite this, no information could be exchanged faster than the speed of light, so relativity was safe. There is no faster-than-light communication.

At its core, entanglement is a correlation between separated objects that is greater than is classically possible. What made it spooky to Einstein was that the correlations were instantaneous, with a measurement on one object immediately determining aspects of the state of the other. This seemed to violate causality, a foundation of Einstein's theory of relativity.

With the award of the CDQI to four exceptional academic research teams and the large influx of talent to ARL, the Army took the lead in developing this most nascent aspect of QIS, the quantum network. Given that quantum information will have to reside on multiple nodes, and the architecture of each node could be different from one to another, for example, ions in one case, trapped neutral atoms in another, defects in solids in yet another, or quantum dots or superconducting qubits in still others, research needs to focus on both interconnecting and translating these different forms of quantum information and maintaining coherence in the process. This press release discusses two novel schemes for transferring quantum information using both photons (light) and phonons (sound). As platforms for quantum information, these are distinguished as "flying qubits," or the carriers of quantum information in a network. Necessary for maintaining the coherence and distributing entanglement across large distances are going to be quantum repeaters, quantum memories, and quantum protocols such as quantum teleportation as a way to move quantum information from place to place. What the CDQI Chicago team has achieved and described here is a novel way to distribute quantum entanglement, and even more impressively, a quantum state. Particularly amazing is that they could transfer the state without ever occupying the intervening communication channel! This has enormous potential for efficient transfer of information across quantum networks. Fundamental progress such as this made by the CDQI and ARL in-house researchers over the past five years firmly established them as leaders in developing this extremely Army-relevant research area.

As already mentioned, a quantum network doesn't replace an ordinary network for communication or computing—it's distinct. So what benefits do quantum networks provide? The benefits lie in what entanglement enables. An often-cited use is in secure communication. How to do this effectively is still an active area of research, as one wishes security protocols that are multipartite and authenticated. (The most widely known example of quantum communication is neither; it is point-to-point quantum key distribution, which is not an application of a quantum network.) But there are known authentication and security protocols (secret sharing, Byzantine agreement, quantum money, and others) that can be implemented on a quantum network. They are interesting but remain more curiosities than useful applications. On the other hand, there are known useful, non-communications applications for quantum networks, including distributed quantum computation, blind quantum computation, distributed clock synchronization, and distributed quantum sensors. The latter are of particular interest to ARL. For example, using coherent quantum data across a network enables improved sensitivity and the ability to extract higher-order moments (like gradients) without loss of sensitivity arising from subtracting noisy data. Related to this, one can get improved imaging resolution in a coherent version of very-long-baseline interferometry. Recently, and tantalizingly, it has been discovered that one can also, in principle, perform computations in computational complexity classes previously deemed impossible by using entangled information sharing across quantum computers.

The DoD's foundational role in investment in QIS created a field that has, in recent years, been widely written about even in the popular press (e.g., The Economist). It did not escape the attention of Congress or the White House either (through the Office of Science and Technology Policy [OSTP]), and in 2018 the National Quantum Initiative (NQI) was launched. In numerous reports, the National Academy of Sciences has acknowledged the DoD's role in laying the groundwork for this. NQI takes QIS to the next level, infusing funding, involving OSTP and all the national science agencies in coordination of efforts, and encouraging a scientific and engineering ecosystem to mature QIS, while recognizing that the field must be guided by science first, as even now, there is much more basic research needed. The Department of Energy (DOE), a new player in the QIS ecosystem, decided that its role is to create a "quantum internet." As this is little else than the quantum network idea ARL has been working on for the past five years, DOE is building on ARL's foundation. In just the last few months, DOE invested in five new centers focused on different aspects of the quantum network. As such, some of ARL's efforts have transitioned, but our foundational research in quantum networks and distributed quantum information continues. In parallel, ARL has also been expanding its focus to quantum sensing and quantum inertial measurement (to augment or replace GPS in denied environments). Yes, QIS enables this too.

QUANTUM OPTICS PROGRAM

Program Manager
Dr. James Joseph

Dr. Joseph completed his undergraduate and graduate studies at Duke University receiving his B.S.E in Physics and Electrical Engineering in 2001 and his Ph.D. in Atomic Molecular and Optical Physics in 2010.

Dr. Joseph started at ARO in 2020 and took over the Optical Physics and Fields Program that was previously managed by Dr. Richard Hammond. He is currently transitioning the program with a focus on quantum optics.

Current Scientific Objectives

1 | Understand how integrated photonics can enhance or enable quantum optics processes for novel capabilities that, if successful, would enable advanced sensing and communication technologies in an optimized size, weight, and power (SWaP) package that can operate in extreme environments and within a contested electromagnetic spectrum.

2 | Enable functionality with light–matter interactions, exploring time-based driven modalities as well as increased interaction strength via cavity quantum electrodynamics enhanced ultra-strong coupling that, if successful, could lead to optically driven solid-state systems that could be utilized for ultra-low energy electronics, quantum computing, or alternate energy.

This success was made possible by:

Dr. James Joseph, Physics Branch

Dr. Joseph Myers, Mathematical Sciences Branch

Citations:

Ball, P. *Nat. Mater.* **19**, 710 (2020).

Cartlidge, E. "Quantum Control Using Laser Light Could Turn Insulators into Conductors and Vice-Versa." *Physics World*. (2020).

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McCaul, G., Orthodoxou, C., Jacobs, K., Booth, G. H. & Bondar, D.I. *Phys. Rev. A* **1010**, 053408 (2020a).

McCaul, G., Orthodoxou, C., Jacobs, K., Booth, G. H. & Bondar, D.I. *Phys. Rev. Lett.* **124**, 183201 (2020b).

"Research shows how to make lead act like gold, enabling optical computing," DEVCOM Army Research Laboratory Public Affairs. (2020).

SUCCESS STORY
Driven Imposters

ARO-funded research at Tulane University and King's College London in collaboration with ARL scientists discovered that shining precisely controlling lasers on a given material resulted in the display of properties from a different substance, which in the long term, could enable a new class of high-speed optical computers. This discovery may also provide avenues to substitute rare compounds with less-expensive and more-efficient electronic components.

CHALLENGE

Originally intended as a study of nonlinear processes of light–matter interactions with a bent toward optical computing applications, this theoretical effort developed a protocol for modifying the optical response of a material by driving it with an external light field. It was soon realized that the framework could be generalized to any property of any material, not just the optical response. Professor Denys Bondar and his team at Tulane University employed what is known as a tracking Hamiltonian. A Hamiltonian is the equation that describes the evolution of a system's properties. The light field is represented by a target function in the tracking Hamiltonian, and once the mathematical representation is worked out, it can be used to guide the system to an arbitrary state. The details are such that Professor Bondar was able to avoid singularities in the trajectories of Hamiltonian, which have been a pitfall of previous attempts at formalizing tracking protocols.

> "The fact that it is possible to control the bulk response of materials in this way may mean that it is possible to control more complex aspects of material behavior. It would be tremendously useful, for example, if one could use this kind of control to induce responses that mimic exotic properties such as superconductivity at high temperatures."
>
> – Professor Bondar, Tulane University (ARL, 2020)

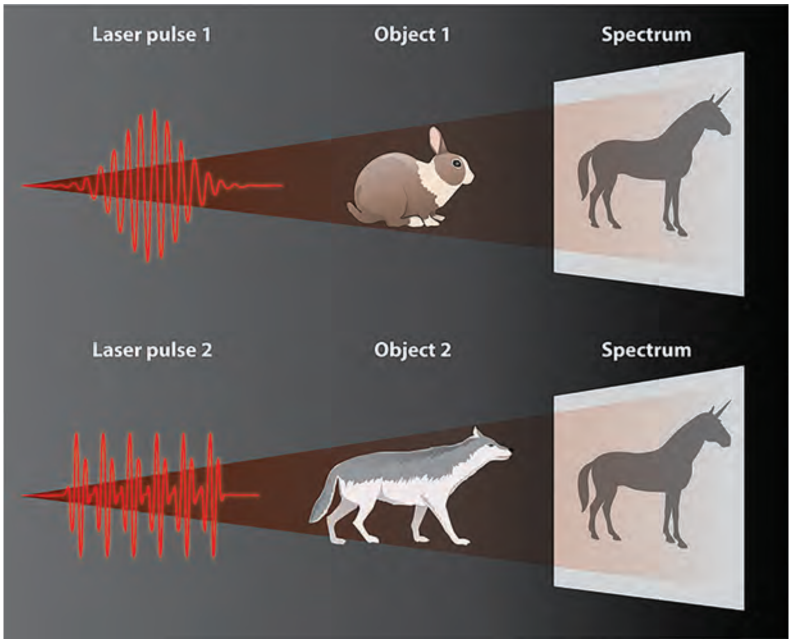


Figure 1: With a newly proposed spectral mimicry scheme, researchers could make two different materials mimic each other's spectra—or produce the spectrum of other, more-exotic materials. Figure and caption adapted from Gorlach et al. (2020).

ACTION

The award was collaboratively funded by former Program Manager Dr. Richard Hammond and ARO Computational Mathematics Program Manager Dr. Joseph Myers. The effort originally envisaged a way to understand nonlinear photonics in the context for optical computing. In the attempt to tailor an optical response, the research team realized that their work had broader application. It was also discovered that material properties can be arbitrarily driven by external fields, so Drs. Hammond and Myers encouraged this new direction of study. Professor Bondar's research was also brought to the attention of ARL personnel, leading to a collaboration between Bondar and Dr. Kurt Jacobs of ARL SEDD on this effort. Together, Dr. Jacobs and Professor Bondar demonstrated how light is converted into an electrical force and produces a tailored response not easily found in nature. These results were published in two articles co-authored by ARL and academic researchers (McCaul et al., 2020a, 2020b).

RESULT

In a landmark result, the team at Tulane University, in coordination with researchers at King's College London and ARL SEDD, developed a procedure to use terahertz fields to drive a material system across a quantum phase transition (Figure 1). Specifically, they showed that using the 1D Fermi Hubbard model (one way to describe a solid-state system mathematically) with the additional terms of the light field modulated correctly causes the materials properties to transition from a Tomonaga–Luttinger liquid (superconducting) phase to a Mott insulator (insulating) phase. Additionally, the researchers demonstrated how to generate an arbitrary spectral response in materials on demand. The system is driven such that the expectation value of the current is in a state associated with certain spectral features, namely, high harmonic generation (HHG). HHG is a nonlinear effect important in ultrafast laser technologies. These results were published in peer-reviewed journals (Ball, 2020; Gorlach et al., 2020) and highlighted in popular scientific media (Cartlidge, 2020).

WAY AHEAD

The next step is to demonstrate a successful application of a tracking protocol in a physical system, as well as explore theoretically ideal test cases. If successful, it may no longer be necessary to search and design materials with specific properties. Instead, common materials could be optically driven to provide the functionality required for a given application.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

Results

- Published two academic papers in *Physical Review*.
- Research featured as highlights in *Physics*, *Physics World*, and *Nature Materials*.
- Established collaboration between ARO-funded academic researchers and ARL SEDD scientists.
- Discovered a new method to create light–matter interactions, which are being explored further by ARO Program Managers.

Anticipated Impact

Controlling material properties such as the superconducting transition temperature could lead to the development of a new class of ultra-low-energy electronics. Further, the controlling spectral response of materials has implications for both advanced sensing and detection avoidance.

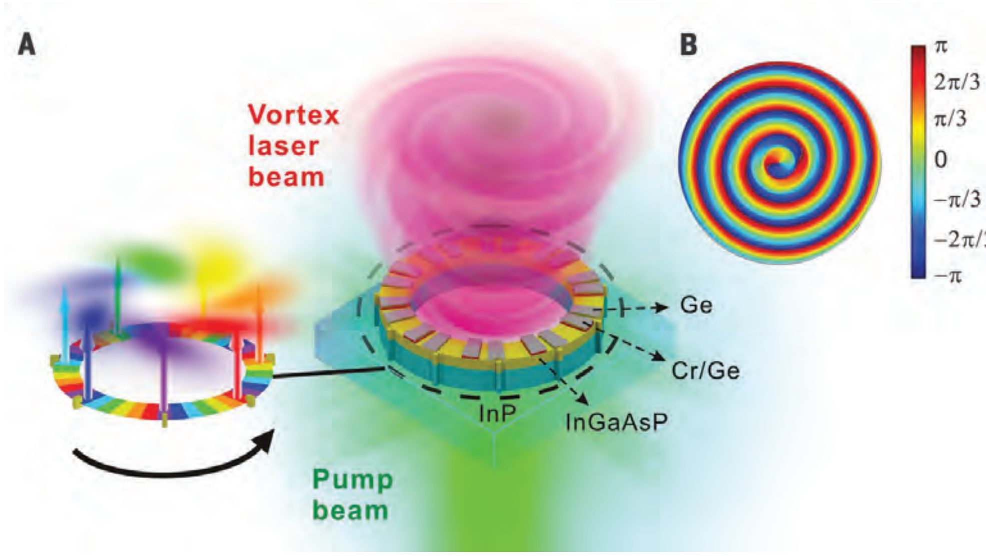


Figure 2: (A) Schematic of the OAM microlaser. The diameter of the microring resonator is 9 μm, the width is 1.1 μm, and the height is 1.5 μm. Lasing occurs in the upward direction, creating an OAM vortex emission with a helical wavefront. (B) Simulated phase distribution of emitted light. A spiral phase map for an OAM charge-one vortex is clearly demonstrated. Figure and caption adapted from Miao et al. (2016).

This success was made possible by:

Dr. James Joseph, Physics Branch

Citations:

Miao, P. *et al*. *Science* **353**, 6298 (2016).

"Penn Engineers Develop First Tunable, Chip-based 'Vortex Microlaser' and Detector, Encode Information in Twisting Beams of Light," *Penn Engineering*. (2020).

University of Pennsylvania. "First tunable, chip-based 'vortex microlaser' and detector." *Science Daily*. (2020).

"Vortex Microlaser' Encodes Information in Twisting Beams of Light," *Duke University Pratt School of Engineering*. (2020).

Zhang, Z., *et al*. *Science* **368** (2020).

SUCCESS STORY

Vortex Microlaser

Two ARO-funded principal investigators, Professor Liang Feng at the University of Pennsylvania and Professor Natalia Litchinitser at Duke University, have collaborated to develop a new type of laser, known as a vortex microlaser, which can manipulate the orbital angular moment (OAM), or twist, associated with the laser light field (Figure 2). The technology will enable increased data transmission in optical communications devices, a novel way to meet the ever-increasing need for higher-capacity information transfer.

CHALLENGE

Information encoding in optical communications is generally accomplished by modulating either the amplitude or frequency of a light field, and the signal is sent either in free space or via an optical fiber. The revolution of fiber-optics communication cannot be overstated and has allowed for significant advances in technology utilizing data on a scale unimaginable just a few decades ago. Unfortunately, the limits of this technology have been reached; new ways of transmitting information must be developed to enable future capabilities requiring an even greater amount of data light machine learning and artificial intelligence. This research effort seeks to use a light field's polarization and phase to increase information capacity in optical data transfer.

"Our findings mark a large step toward launching large-capacity optical communication networks and confronting the upcoming information crunch."

– Liang Feng, Assistant Professor of Materials Science and Engineering and Electrical and Systems Engineering, University of Pennsylvania (Duke, 2020)

ACTION

The Quantum Optics (formerly Optical Physics and Fields) Program has been at the forefront in investing in platforms that are designed using non-Hermitian Hamiltonian theory. These designs usually consist of taking advantage of periodic structures of materials with complex gain and loss properties. There have been a number of successful demonstrations, including one result that was highlighted in an FY19 ARO Year in Review article on the application of non-Hermitian design concepts to laser arrays resulting in greater single-mode output power. This year's highlight was funded when Dr. Joseph decided to increase investment in this space after seeing initial promising results from previous investments. Both Professors Feng and Litchinitser received awards to explore the functional space for non-Hermitian optical devices after early indications signaled promise.

RESULT

The collaborative University of Pennsylvania and Duke University team's breakthrough achievement was the creation of a microring OAM laser that can switch between OAM states on demand in a compact, integrated platform (Figure 3). Generation of complex OAM beams usually relies on free-space optics such as spiral phase plates. Here, the researchers have taken a different approach. The laser is an integrated device comprising gallium arsenide (GaAs) structures. The design of these structures takes advantage of non-Hermiticity, wherein complex refractive-index modulation in the physical structure forms an exceptional point (EP). The EP formation is essential for obtaining robust unidirectional laser emission. The gain properties of the material system can then be driven by external fields to hop the laser between OAM modes. Each OAM mode represents an additional dimension of information space that, in conjunction with frequency and amplitude modulation, could, in principle, geometrically increase the information capacity of optical communications.

WAY AHEAD

Many paths remain to be explored, including creating efficient channels for the propagation of OAM light and integration to modern fabrication processes. Also intriguing is the application of OAM modes to quantum technology. OAM modes are orthogonal and therefore offer an infinite Hilbert space in which to manipulate quantum information. If successfully refined, this novel capability would be a good candidate for more applied research funds and rapid technology transfer.

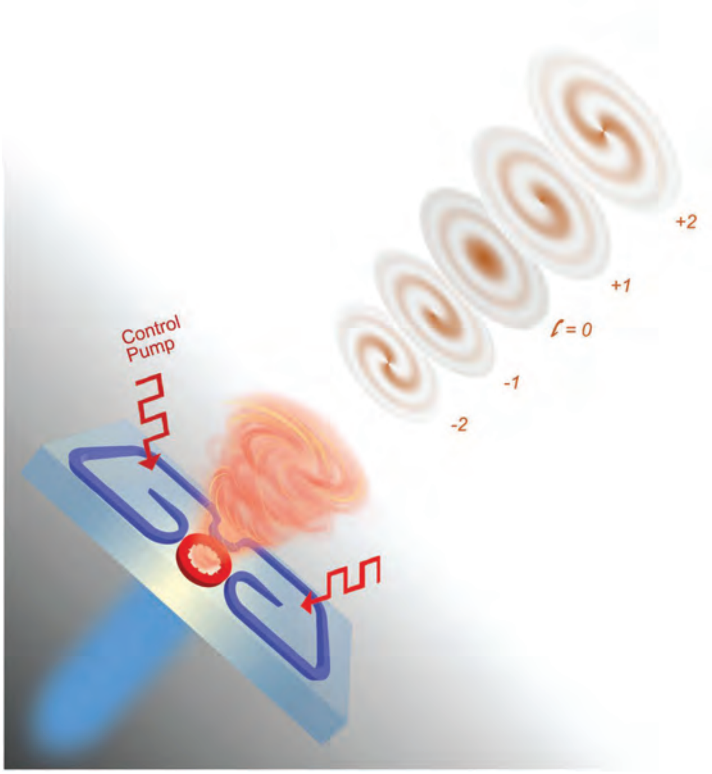


Figure 3: Asymmetry in optical "pumping" from the control arms on either side of the microring laser allow for resulting light's OAM to be "tuned" to different modes. Figure and caption adapted from Zhang et al. (2020).

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Network Science and Computational Sciences

Results

- Published academic papers in the journal *Science*.
- Work featured as highlights in *Science Daily*.
- Results led to new potential collaborations beginning in 2021 to drive studies in hyperentanglement for potential future Army applications in quantum networks.

Anticipated Impact

This result has the potential to revolutionize optical information transfer by providing a robust and efficient method of encoding information in the twist associated with the laser light field.

SOLID STATE PHYSICS PROGRAM

Program Manager
Dr. Marc Ulrich
Chief (Acting), Electronics Branch

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University, receiving his Ph.D. in Condensed Matter Physics in 2001.

He came to ARO in 2003 as the Program Manager for what was then called Condensed Matter Physics and was promoted to the additional role of Chief, Physics Branch, in 2008. He transferred from Chief, Physics Branch to Chief, Electronics Branch in 2020.

Current Scientific Objectives

1 | Achieve ultra-strong coupling between light and matter to fundamentally alter the physics of the solid-state system that, if successful, will enable future technologies in sensing and information processing.

2 | Determine how resistance-free current can be obtained at ambient conditions without relying on superconductivity that, if successful, will enable dramatic reductions in the energy required for electronic information processing.

3 | Understand the physics governing the interaction between topological and magnetic states that, if successful, is anticipated to lead to ultra-efficient electronics in support of Intelligence, Mission Command, and Maneuver Functional Concepts.

This success was made possible by:

Dr. Marc Ulrich, Physics Branch

Dr. Joe Qiu, Electronics Branch

SUCCESS STORY

Rich Interactions between Topological and Magnetic States

ARO-funded work at the Massachusetts Institute of Technology (MIT) has determined that chromium sesquitelluride (Cr_2Te_3) is a promising material for determining the magnetic/electronic interactions at the interface between magnetic and topological materials. These findings may enable future electronics that exceed the energy efficiency of today's technologies, thereby opening the door to ultra-low-power electronics.

CHALLENGE

Theoretical studies have determined that coupling between magnetism and topological insulators may provide a route to ultra-efficient electronic information processing. Topological insulators are a relatively new discovery in which the relationship between an electron's energy and momentum is twisted compared to normal (trivial) materials. This twisting ensures that there are electron conduction paths at the surface (called topological surface states) that are not destroyed by defects. The efficacy of these studies depends on the interactions at the interface between the magnetism and the topological surface states. However, the precise mechanisms that define the dance between the magnetism and the topological surface states are currently unknown.

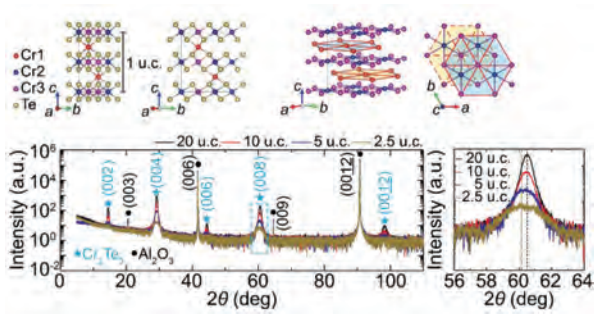


Figure 1: Top: The crystalline structure of Cr_2Te_3 as seen from various angles. Note the Cr/Te layers that are separated by layers of sparse Cr (red). Bottom: X-ray diffraction measurements of various thicknesses of Cr_2Te_3 grown by molecular beam epitaxy. Bragg peaks expected for Cr_2Te_3 are shown in blue. To the right is a zoom into the (008) Bragg peak. Courtesy of the Moodera laboratory.

ACTION

The Solid State Physics Program and ARL SEDD have been working together on topological materials for over a decade. Dr. Ulrich's emphasis in the Solid State Physics Program on electronic correlations in nascent topological materials, along with the laboratory's emphasis on phenomena operative at elevated temperatures strategically, drove investments in magnetic correlations. Perceiving the central role of the interfacial magnetic interactions and the challenge within the community to readily verify the nature of those interactions, Dr. Ulrich sought out experts in the community to seek answers regarding the magnetism at the interface between magnetic and topological materials and how it interacts with the topological surface states. One of these experts is Dr. Jagadeesh Moodera at MIT. Dr. Ulrich selected Dr. Moodera because of his extensive history and knowledge regarding magnetism, interfaces, and materials growth, and previous work on magnetic/topological interfaces that revealed unexpected behavior. Dr. Ulrich awarded Dr. Moodera's proposal as a cooperative agreement and worked with ARL SEDD to hire and place an ARL postdoctoral scholar in Dr. Moodera's laboratory to collaboratively augment the work.

RESULT

Cr_2Te_3 is a quasi-two-dimensional ferromagnet that has been rediscovered in the last 2-3 years. Interest in this material resurged because its unique structure indicates that it may be feasible to utilize it as a ferromagnet in its monolayer limit. Many topological materials are tellurides, suggesting that the magnetic exchange interaction might be stronger, because tellurium is common to both materials. Ultra-thin ferromagnetic films may be ideal for topological electronic devices (TEDs) involving magnetism. If the interaction can be made strong enough, biasing the magnetic–topological interface can efficiently switch the magnetic order of the magnetic material.

There is a long road between a chemical formula with an idealized crystalline structure and a real material. Much of this year's progress has been in developing the growth procedures for $Cr_2Te_3$and determining the resultant crystalline quality and magnetic properties. Dr. Moodera and Dr. Hang Chi, an Oak Ridge Associated Universities (ORAU) Fellow, deposited Cr_2Te_3 by carefully controlled molecular beam epitaxy on several substrates. Reflection high-energy electron diffraction measurements during the growth confirmed layer-by-layer growth of the films. Films were subsequently studied extensively by x-ray diffraction and electron microscopy to analyze the crystalline nature of the films. Figure 1 shows the crystalline structure and x-ray diffraction revealing the expected diffraction for Cr_2Te_3. Optimal growth resulted in the correct Cr_2Te_3 phase revealing sparsely occupied Cr layers between $CrTe_2$-type layers.

Upon having established the growth conditions for high-quality Cr_2Te_3, the magnetic properties of films of several thicknesses were studied in depth. This finding establishes a baseline for understanding the interaction between the magnetism in Cr_2Te_3 and a topological insulator. It is hoped that a voltage across or current through a topological material would change the magnetism of Cr_2Te_3. Figure 2 shows the magnetic characteristics of a 20-unitcell-thick sample at temperatures between 10 and 160 K. These studies revealed a rich magnetic structure. The easy axis was confirmed to be along the growth axis (the c-axis of the crystalline structure) with the expected Curie temperature of 160 K. At low temperatures, there is a strong magnetic hysteresis with features that suggest that the material is more than merely a ferromagnet. Magnetotransport studies in which Hall resistance in a Hall bar device is studied as a function of magnetic field revealed the nature of this material more fully. Also shown in Figure 2, the magnetotransport revealed an anomalous Hall effect, which switches sign with temperature and an extra dip and bump at 10 K. The anomalous Hall effect (AHE) in imperfectly conducting ferromagnets has been known for many decades. Recently, physicists have clarified that the AHE can be intrinsic—due to purely band structure curvature known as Berry curvature—or extrinsic—due to an imbalance in scattering of electrons off defects to the left versus right. That the AHE changes sign with temperature suggests that both intrinsic

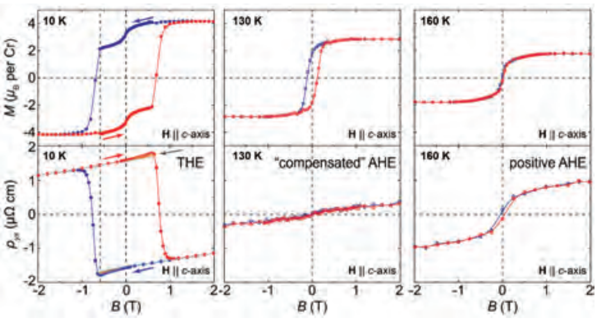


Figure 2: Magnetic properties of 20 u.c. Cr_2Te_3. Top panels: magnetization as a function of external magnetic field at 10, 130, and 160 K. The ferromagnetic response is revealed by the hysteresis, which closes at the Curie temperature: 160 K. Bottom panels: Hall resistance as a function of external magnetic field for the corresponding temperatures. The black arrow labeled "THE" in the lower-left panel shows the extra bump revealing the topological Hall effect. Courtesy of the Moodera laboratory.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Results

- Discovered the topological effects in a thin-film magnet.
- Results submitted for publication.
- Transitioned the knowledge of the discovery to ARL researchers for subsequent studies in TEDs.

Anticipated Impact

The discovery of an unexpected electronic effect in Cr_2Te_3 enriches studies into the interplay between magnetic and topological materials, and may reveal new opportunities for energy-efficient information processing.

and extrinsic effects are in play with each taking the dominant role in different temperature regimes. The extra dip and bump at low temperature is a renowned telltale sign of the presence of magnetic vortices, dubbed skyrmions. These vortices are topological defects in the magnetic structure of the material revealing that Cr_2Te_3 itself has topologically interesting properties—independent of whether or not a topological insulator may be present.

WAY AHEAD

As the first results on Cr_2Te_3 indicating these properties, the Solid State Physics Program continues to invest in unraveling the magnetic personality of this material. It is bound to be all the more interesting when it is wed with a topological insulator. Just what will the nature of that relationship be? Regardless of the outcome, having a deeper understanding of the interfacial interactions will provide valuable knowledge that can be applied to the design of magnetic–topological device concepts.

This success was made possible by:

Dr. Marc Ulrich, Physics Branch

Citations:

Wu, X. *et al. Nat Commun* **11**, 4532 (2020).

SUCCESS STORY

Transition Physics Between Topological States Revealed

This ARO initiative has revealed the detailed physics of the transition between 2D magnetic and electronic phases. Knowledge of the nature of transitions such as these will be essential for the advancement of initiatives to devise electronic devices based on topological materials, potentially leading to ultra-low-power electronics.

CHALLENGE

Superconductivity is not the only way for electrical current to flow without resistance. The quantum Hall effect (QHE) discovered in 1980 is another, but can only exist at temperatures near absolute zero and in very high magnetic fields. A recent discovery of a related effect, the quantum anomalous Hall effect (QAHE), revealed that the magnetic field is no longer necessary for resistance-free current. If materials quality can be improved and interactions between magnetism and electrons better understood in pertinent material systems, this effect might be brought to room temperature, providing an alternative route to resistance-free current at ambient conditions.

ACTION

Shortly after the 3D topological insulator (TI) was discovered, Dr. Ulrich recognized the potential impact of the field toward future Army-relevant applications. He began investing in topological materials and the unique physics therein using core funds and competing a successful topic to initiate multidisciplinary studies on topological materials via an ARO Multidisciplinary University Research Initiative (MURI).

Within the Topological Materials MURI, it was discovered that topological states are not as rare as originally thought. Potentially, a fourth of all known crystalline materials host topological states. Generically speaking, a topological material is one in which the electronic structure governing the behavior of electrons in the material has a non-trivial twist. Though such a material may be a perfectly good insulator, the interface or surface with another material (even air) forces a conducting state at the interface. This so-called topological surface state has unique properties that many are seeking to exploit for possible technological opportunities. In a 2D topological material, the interior is insulating but electrons can travel along one-dimensional conducting edge channels. A quantum Hall insulator formed by a sheet of electrons in a strong magnetic field can be considered a special topological material in which the edge-state current can propagate clockwise or counterclockwise with zero resistance. Of particular interest is the related QAHE, because it hosts the same perfectly conducting edge states while eliminating the need for an external magnetic field.

One of the advances enabled in part by the Topological Materials MURI was the experimental realization of a related topological state referred to as an axion insulator (AI). An AI is almost exactly like a QAHE except that it includes a type of magnetism that eliminates the conducting edge states. This work was conducted in 2018 at The Pennsylvania State University by co-principal investigator, Dr. Nitin Samarth, a new faculty member, Dr. Cui-Zu Chang, and their research teams. This state is fully insulating and enables studies of the coupling between magnetism and electrons in topological materials. These effects in topological materials are expected to far exceed magneto-electric coupling of any other known mechanism. At the time that this work was being published, Dr. Chang reached out to Dr. Ulrich with the idea of increasing the temperature at which QAHE is operative and understanding the scaling behavior of physics in the QAHE regime. This concept was strategically related to the goals of the Solid State Physics Program. After extensive discussions regarding the details of how magnetism was creating the various states, Dr. Ulrich encouraged a proposal, which was subsequently funded.

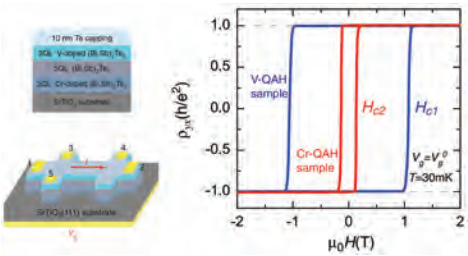


Figure 3: The QAHE. The edge resistance (ρ_{xx}) goes to zero for certain magnetic fields—including a zero magnetic field. This is one step closer to zero resistance at ambient conditions. While low temperatures are still required for today's materials, no externally applied magnetic field is necessary. From Wu et al. (2020).

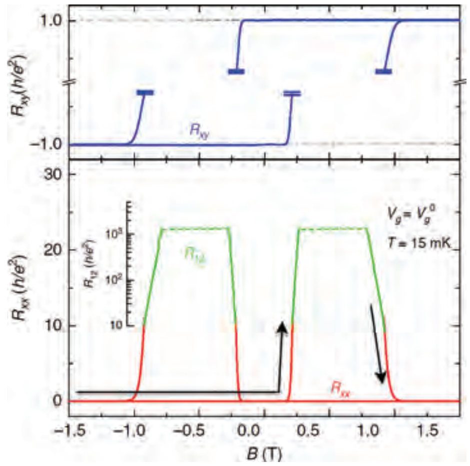


Figure 4: The magnetic/TI/magnetic sandwich and tuning between the QAHE and AI states. The resistance across the Hall bar (R_{xy}) is quantized to h/e^2. The edge resistance (R_{xx}, lower graph) is either zero or approaches infinity. As the magnetic field is raised to about 0.4 T, only the V-doped layer switches magnetization creating the highly resistive AI state until about 1.2 T at which the Cr-doped layer switches also, recreating the QAHE again. From Wu et al. (2020).

RESULT

Among many published results was the recently published work in which Dr. Chang, his research team, and collaborators revealed the nature of the quantum phase transition between the QAHE and AI in a single magnetic TI heterostructure. This was enabled by the development (within the Topological Materials MURI) of a unique tricolor sandwich (that is, one in which the top and bottom pieces of bread are different) of topological materials. The QAHE can be designed by sandwiching a thin 3D TI between two ferromagnetic materials. Magnetic fields or the presence of magnetic ions near the TI surfaces in which the N-S direction of the magnet points into the surfaces destroy the topological surface state. A magnetic/TI/magnetic sandwich in which the magnetization of the outer layers points in the same directions—that is, the N-S direction of top and bottom layers are the same—leaves the edges conducting. This is a QAHE. Electrical measurements of such a system reveal a zero-resistance state along the edges of the sample. Tuning an external magnetic field during electrical transport measurements demonstrates the QAHE (Figure 3). While this is similar to the QHE, the underlying mechanism is fundamentally different; the magnetic ions do not simply provide an external magnetic field, they completely alter the relationship between energy and momentum of electrons in the TI.

To achieve the AI state, the N-S magnetism of the top and bottom surfaces must point in opposite directions. This is a non-trivial endeavor as external magnetic fields are virtually the only robust way to control the magnetization of a material. Dr. Chang, however, exploited knowledge of two separate magnetic dopants to overcome this limitation. The ternary TI, $(Bi,Sb)_2Te_3$ (BST), was chosen because it is of sufficient quality. Dilute magnetic forms of BST are ideal magnetic materials for the sandwich to ensure chemical compatibility between the materials and high-quality interfaces. From previous experiments Dr. Chang knew that QAHE could be obtained in both Cr-doped and vanadium (V)-doped BST. Since the Cr- and V-doped films have a magnetic saturation at different external magnetic fields, a sandwich of these materials could be tuned to have N-S magnetization of the two films parallel or anti-parallel, thus enabling both the QAHE and the AI state in the same structure. Figure 4 shows the results.

With a single sample hosting both the QAHE and AI, the physics of the quantum phase transition could be studied in detail. These kinds of detailed studies are essential to fully comprehend—and thus engineer or optimize—the interactions between magnetism and electrons in topological materials. The team discovered that right at the transition—with the N-S magnetization of one surface stably pointing opposite the external magnetic field and the other flipping to point along the external field—the topological surface state proximal to the transitioning magnetic material comprises puddles of QAHE and AI. At the edges between these puddles are edge states that interact at four-fold points where the current goes in on two axes and out on two others. Remarkably, this physical process is identical to transitions within the QHE, even though the underlying QHE and QAHE mechanisms are different.

WAY AHEAD

Both the QAHE and AI states have interesting possibilities for concepts such as information processing and sensing modalities. Determining if the yet-to-be-envisioned ideas are meaningful will require the expansion of materials hosting these states, additional studies of the physics governing the phenomena, and increasing the temperatures where they are active to more-relevant temperature regimes. The Solid State Physics Program anticipates continued investments to accomplish this goal.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Results

- Discovered the physical mechanism driving a system between admitting a current with zero resistance and having an infinite resistance, which may enable future ultra-low-power information processing or novel sensing modalities (Wu et al., 2020).

Anticipated Impact

If 2D topological electronic phases can be stabilized at ambient conditions, it provides a route to electronic device interconnects that greatly exceed the efficiencies of copper and gold. Inductors, memory, and other electronic devices would benefit, with reduced power requirements for communications, radar, and information processing.

INSTITUTE FOR COLLABORATIVE BIOTECHNOLOGIES

Program Manager
Dr. James Burgess

Dr. Burgess completed his undergraduate studies at Longwood College, receiving his B.S. in Chemistry. He earned his Ph.D. in Chemistry from Virginia Commonwealth University in 1997 before serving as a postdoctoral research associate at Ames Laboratory, the U.S. Department of Energy's National Laboratory administered by Iowa State University.

He joined ARO in 2019 following faculty appointments at Case Western Reserve University and Augusta University, where he served as Chair of the Department of Medical, Laboratory, Imaging and Radiologic Sciences in the College of Allied Health Sciences.

Current Scientific Objectives

The ICB is one of the Army's University Affiliated Research Centers (UARCs). The ICB's core research goals are organized into three research focus areas that together aim to understand and control biological processes, and use or adapt them for novel technologies that enhance Warfighter capabilities and performance:

1 | *Systems and Synthetic Biology* pursues four interrelated research themes: understanding biological networks and circuits, biological synthesis strategies, spatial and temporal dependences in biological systems, and manipulation of cellular behaviors. These projects engineer novel biological pathways that, if successful, can be used to synthesize strategic materials to provide high-sensitivity sensing and monitoring, and optimize the Warfighters' microbiome.

2 | *Biologically Enabled Materials* focuses on three core research themes: biochemical syntheses of new materials, biotic-abiotic interactions and interfaces, and integration of biological components in materials that function under abiotic conditions. These efforts, if successful, will impact new capabilities for portable energy applications, point-of-need syntheses of strategic materials, and lightweight, functional materials for signature management.

3 | *Cognitive Neuroscience* investigates the core components of human cognition that are essential for successful performance in complex environments. This effort, if successful, aims to tackle the fundamental challenges a Soldier faces in real-world operational planning, navigating, decision-making, and sustaining task prioritization and situational awareness as information complexity and stress escalate.

This success was made possible by:

Dr. Robert Kokoska,
Life Sciences Branch

Dr. James Burgess,
Physical Sciences Division

Citations:

"DoD Approves $87 Million for Newest Bioindustrial Manufacturing Innovation Institute" *Department of Defense* (2020).

Furubayashi, M. *et al. Adv. Funct. Mater.* 2004813 (2020).

SUCCESS STORY

Genetic Tuning of Magnetic Iron Oxide Nanoparticle Size, Shape, and Surface Properties in *M. magneticum*

Synthetic biological protocols for the reliable production of genetically tuned magnetic iron oxide nanoparticles by *M. magneticum* have been finalized at the Massachusetts Institute of Technology (MIT) under support from the ICB UARC. These results have transitioned to ARL and industry to produce nanoparticles for satellite communications antennas. Novel methods were developed to tune the expression levels of nine magnetosome-associated proteins, several protein "handles" for morphology control were discovered, and novel techniques to produce silica-encapsulated or fluorescent magnetic nanoparticles with shells of tunable thickness were invented.

CHALLENGE

Iron oxide nanoparticles are useful in many nanotechnology applications including as contrast agents, magnetic inks, sensors, and data storage substrates. Their end-use application dictates the size, morphology, and other properties that the particle needs; magnetic properties, for example, are directly related to the size of the particle, with particles smaller than 130 nm exhibiting single-domain ferromagnetism and particles smaller than 30 nm only showing superparamagnetism. Traditional chemical synthesis techniques produce particles with wide distributions in size and shape, the heterogeneity of which render them unsuitable for many applications.

Biogenesis of magnetic particles, however, is widely found in nature, with certain magnetotactic bacteria known for producing chains of magnetite particles with tight particle size and shape distribution known as magnetosomes. The goals of this ambitious project were to render *M. magneticum* genetically tractable by genetically engineering promoters; create inducible systems for control of magnetite production proteins; test the morphology of particles produced in magnetosome overexpression strains; and generate novel encapsulations of magnetite particles via surface display (Figure 1).

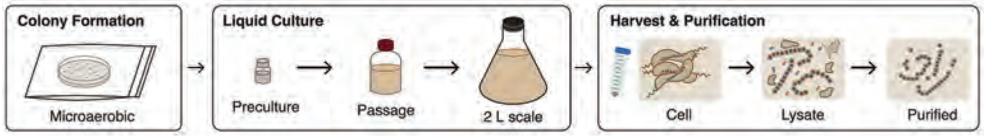


Figure 1: *M. magneticum* colony formation, liquid culture scale-up, and subsequent harvest and purification steps for magnetosome production. Figure adapted from Furubayashi et al. (2020).

ACTION

In 2012, ARL HRED made a recommendation that the ICB Cognitive Neuroscience team include studies that addressed the cognitive effects of individuals under conditions of physical stress. In response to this Army need, former UARC Program Manager, Dr. Robert Kokoska, saw an emerging opportunity for the Army when Professor Christopher Voigt, who was a young assistant professor in the then-nascent field of synthetic biology, joined the faculty at MIT, which is one of the three campuses comprising the ICB UARC. Dr. Kokoska encouraged Professor Voigt to submit a proposal to ARO via the ICB, and his ambitious, high-risk ICB project, "*Synthetic Biology: Refactoring the Genetics of Metal Nanocluster Synthesis*," was chosen for initial funding in 2012.

This was the first true "synthetic biology" project that was funded under the Army's ICB UARC, and work on it began more than three years prior to the publication of the January 2015 "DoD Research & Engineering Technical Assessment on Synthetic Biology," which stated, "because of the existing and promising future capabilities of engineered organisms, this assessment finds that the synthetic biology space presents a major opportunity for DoD." Since 2012, the ICB has provided continuous support for a sequence of evolving synthetic biology investigations that have been led by Professor Voigt and have benefited from sustained collaborations with scientists from the ARL, up to and including his currently funded project "Synthetic Biology as a Route to New Composite Nanomaterials with Unique Optical/Electronic/Photonic Properties." This continuous, longitudinal funding over eight years through the ICB has resulted in following achievement of the ambitious vision that Professor Voigt proposed to the ARO Program Manager and ICB UARC co-Directors in 2011:

> *Chemical routes for producing metal nanoclusters have several challenges, including: (i) control of size and shape, (ii) precision of atom placement and imperfections, (iii) low yields and high-cost separations, and (iv) toxic byproducts. In contrast, many relevant nanoclusters are produced in nature and these enzymatic pathways are highly precise. They would enable the access to new crystal growth patterns not possible with bulk chemistry. The challenge is that these pathways consist of many genes (up to 100) whose expression levels require careful regulation. To address this problem, we will apply tools from synthetic biology to refactor these pathways in order to build a genetic platform of engineering and optimization. Refactoring is a process by which the complex natural genetics encoding a biological function are replaced by synthetic, well-characterized parts to create a system whose genetics are completely defined.*

RESULT

Protocols for the reliable production of iron oxide nanoparticles by the magnetotactic bacteria *M. magneticum* have been finalized at MIT under support from the ICB UARC and have been transitioned to ARL. These protocols are being used as part of an ongoing collaboration with industrial partners Lockheed Martin and White Dog Labs to produce nanoparticles for use in satellite communication equipment antennas.

This ICB-funded work has resulted in a peer-reviewed journal article in *Advanced Functional Materials* (Furubayashi et al., 2020) that acknowledges ARO funding via the ICB and credits Drs. Justin Jahnke, Brendan Hanrahan, and Dimitra Stratis-Cullum of ARL as co-authors (Figure 2). The ARL scientists were responsible for determining the difference in material properties of the magnetosomes that were produced by the wild-type and genetically engineered magnetotactic bacteria using both Fourier transform infrared and x-ray photoelectron spectroscopy. There is an additional personnel connection with the ICB to note: Dr. Jahnke completed his doctorate at the University of California, Santa Barbara under the training of Dr. Bradley Chmelka, the co-Director of the ICB, prior to joining ARL.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Biological and Biotechnology Sciences

Results

- Published an *Advanced Functional Materials* article co-authored by Army, academic, and industrial researchers in October 2020.
- Transitioned protocols for bio-production of magnetic iron oxide nanoparticles to ARL.
- Developed technology through the ICB UARC project that has now been selected as the basis for the initial quick-start scale-up project for the BioMADE DoD Manufacturing Innovation Institute.

Anticipated Impact

Synthetic biology-sourced magnetic iron oxide nanoparticles are expected to provide advances in high-frequency satellite communications, permanent memory, power transformers, and supercapacitors.

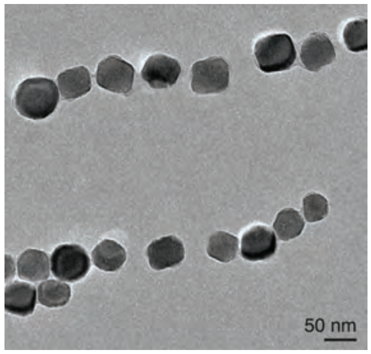


Figure 2: Transmission electron microscopy image of the purified magnetosome nanoparticles after optimizing growing conditions. Figure and caption adapted from Furubayashi et al. (2020).

WAY AHEAD

The results of Professor Voigt's ICB UARC basic research project were selected as the basis for a "quick-start" scale-up project, "Bio-Manufacturing Nanoparticles for Antenna, Transformers, Supercapacitors, and Stealth Coatings," which was included within the July 2020 BioIndustrial Manufacturing and Design Ecosystem (BioMADE) proposal for the DoD Bioindustrial Manufacturing Innovation Institute competition.

On October 20, 2020, the DoD announced an $87 million, seven-year award to BioMADE, a nonprofit created by the Engineering Biology Research Consortium, for a new Manufacturing Innovation Institute. The BioMADE quick-start project, based on eight years of ICB-funded research, aims to scale up bio-production of magnetosomes to kilogram quantities within one year and 10- to 100-kg quantities in two years for use in technology evaluation and demonstration in multiple defense and civilian applications.

This success was made possible by:

Dr. Robert Kokoska, Life Sciences Branch

Dr. James Burgess, Physical Sciences Division

SUCCESS STORY

Fundamental Understanding of Human Adaptive Cognition during Physical Exertion

The most significant output of this work was the development of sophisticated protocols for measuring differences in human brain activity and behavioral performance on cognitive tasks during physical exertion, under fatigue and stress, and while at rest. Some of these protocols are now being used to support the Army's Monitoring and Assessing Soldier Tactical Readiness and Effectiveness (MASTRE) program, which is focused on developing an understanding of Soldier physiology, cognition, and performance in real-world Army mission scenarios.

CHALLENGE

Coherent and adaptive Soldier performance is supported by the interplay among sensory, perceptual, and cognitive systems that mediate the prioritization of information processing in a manner that balances current objectives and expectations in light of new information from the environment. Importantly, for optimal information processing, priority control must be maintained in the context of the Soldier's current global behavioral state (e.g., locomotion, motivation, arousal, fatigue, sleepiness). A major focus of the U.S. Army Human Dimension Science & Technology strategy has been to develop methods to monitor and detect changes in perceptual and cognitive states in an effort to optimize Soldier performance. In 2016, the Army Science Board determined that Soldier optimization and enhancement technologies are at disparate levels and thus research in this area is needed and, specifically, physical, cognitive, and psychological domains should be targeted. Although past efforts have resulted in some progress, their success has been severely limited, because they have either assumed that global behavioral states (e.g., motivation, arousal, fatigue, sleepiness) have nonspecific effects on perception and cognition or ignored the important and specific role played by global behavioral states in mediating cognition.

ACTION

In 2012, former UARC Program Manager, Dr. Robert Kokoska, invited Dr. Barry Giesbrecht of the University of California, Santa Barbara (UCSB) to submit a new ICB basic research proposal targeting a detailed fundamental understanding of human adaptive cognition under fatigue and stress. That work involved systematic manipulations of human physiological states using sophisticated exercise protocols. Recognizing that understanding optimal Soldier performance requires understanding the interplay between physical states and cognitive function, Dr. Kokoska helped Dr. Giesbrecht navigate the oversight process with the Army Human Research Protection Office and initiate productive research collaborations with Army scientists at DEVCOM SC and ARL that continue to the present.

RESULT

The most significant output of this work was the development of sophisticated protocols for measuring human brain activity and behavioral performance on cognitive tasks during physical activity.

ARL Competencies:

Military Information Sciences

Humans in Complex Systems

The approaches developed by Dr. Giesbrecht and his ICB-supported team at UCSB have opened the door to four novel investigations of human cognition and brain function during physical exertion:

1. *Development of robust protocols for measuring brain activity during physical exertion.* A primary measure of brain activity is scalp-recorded electroencephalography (EEG), which is easily contaminated by movement and sweating. Novel protocols for measuring brain activity and performance during exercise were developed and related to changes to behavior, neuroendocrine markers of stress, aerobic capacity, and brain activity.

2. *Physical exertion affects multiple stages of human cognition.* Many studies have demonstrated consistent effects on higher-order cognitive functioning following exercise. This research discovered that these cognitive functions are also modulated during exercise and observed enhanced sensory responses, suggesting that exercise influences cortical excitability at the earliest stages of information processing.

3. *Physical exertion alters neural coding.* Nonhuman mammalian and invertebrate brains exhibit large increases in the gain of feature-selective neural responses in the sensory cortex during locomotion, suggesting that the visual system becomes more sensitive when actively exploring the environment. Through application of a novel computational method to human EEG data acquired from subjects engaged in a feature-selective attention task during exercise, the nature of exercise-induced gain on feature-selective coding in the human sensory cortex was revealed. This provides valuable evidence linking the neural mechanisms of behavior state across species.

4. *Adaptive cognition is altered by reward.* One's previous experience with reward can enhance subsequent performance in future tasks when previously rewarded information is task-relevant, even though there is no prospect for reward. Importantly, performance is impaired when the previously rewarded information is task-irrelevant. The research team discovered corresponding rapid changes in brain activity, suggesting that the activity of neurons in the visual cortex are altered by previous experience with reward, even when no reward is present.

This work has also led to new discoveries about human cognition at rest. Mental representations of behaviorally relevant visual features and locations are based on information sampled from the environment and can persist in visual short-term memory even in the absence of maintained external sensory input. Dr. Giesbrecht and his team have discovered that these representations are maintained by at least two distinct processes, both mediated by EEG oscillations in the alpha frequency band, and have recently demonstrated that these processes are also robust to physical exertion (Figure 3).

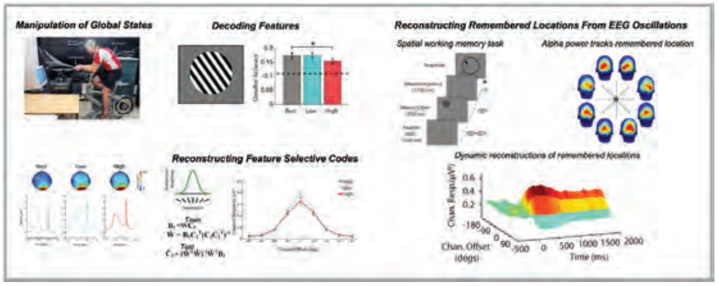


Figure 3: Experimental methods leading to understanding impact of global states and cognitive priority control. Image adapted from the Giesbrecht group.

WAY AHEAD

The basic research support provided by the ARO through the ICB has resulted in the development of cutting-edge capabilities that have allowed Dr. Giesbrecht and his team to respond swiftly to rapidly emerging Army needs. For example, the exercise protocols developed under ICB core funding served as the foundation for new stress protocols that were required to conduct work supported by two subsequent projects that were funded by the Army through the ICB UARC: Biomarkers of Stress States and Rapid, Adaptive Decisions and Recovery from Stress. In both cases, these research programs were heavily informed by input from and consultation with Army scientists.

In 2020, DEVCOM SC has ramped up the multi-domain Army research program MASTRE, which is focused on developing an understanding of Soldier physiology, cognition, and performance in real-world Army mission scenarios. The Army scientists leading this program needed to partner with academic investigators who have the tools and experience for conducting rigorous experiments and comprehensive literature surveys to develop understanding and predictive models about the interaction among locomotion, exertion, attention, and cognition. Because of Dr. Kokoska's foresight in 2012 and the continual support of his work by the ICB UARC over the past eight years, Dr. Giesbrecht and his team were in a perfect position to contribute their skills and expertise to help DEVCOM SC execute MASTRE's important mission.

Results

- Developed robust protocols for measuring brain activity during physical exertion.
- Discovered that physical exertion affects multiple stages of human cognition.
- Discovered that adaptive cognition is altered by reward.

Anticipated Impact

The anticipated impact of these research results and protocols will be seen via the multi-domain Army MASTRE program, which is focused on developing an understanding of Soldier physiology, cognition, and performance in real-world Army mission scenarios.

INSTITUTE FOR SOLDIER NANOTECHNOLOGIES

Program Manager
Dr. James Burgess

Dr. Burgess completed his undergraduate studies at Longwood College, receiving his B.S. in Chemistry. He earned his Ph.D. in Chemistry from Virginia Commonwealth University in 1997 before serving as a postdoctoral research associate at Ames Laboratory, the U.S. Department of Energy's National Laboratory administered by Iowa State University.

He joined ARO in 2019 following faculty appointments at Case Western Reserve University and Augusta University, where he served as Chair of the Department of Medical, Laboratory, Imaging and Radiologic Sciences in the College of Allied Health Sciences.

Current Scientific Objectives

1| Engages Army colleagues to dramatically improve the survivability and capabilities of Soldiers and their platforms by exploring and extending the frontiers of nanotechnology through fundamental research that, if successful, may lead to revolutionary improvements in a wide array of existing equipment and the development of groundbreaking new equipment.

2| With the goal of performing world-class research, actively engages jointly with Army and industry partners to enable efficient transitioning of research that, if successful, will mature swiftly to the higher technology readiness levels suitable for applied research and development by Army labs, defense corporations, and start-up companies.

This success was made possible by:

Mr. John R. McConville, Physical Sciences Division

Dr. James Burgess, Physical Sciences Division

Dr. Henry Everitt, DEVCOM AvMC

Citations:

Wang, F. *et al. Proc. Natl. Acad. Sci. USA*, **115**, 6614-6619 (2018).

Chevalier, P. *et al. Science* **366**, 856 (2019).

Chu, J. "Researchers Generate Terahertz Laser with Laughing Gas," *MIT News Office*. (2019).

SUCCESS STORY
Widely Tunable Compact Terahertz Gas Laser

A collaboration between DEVCOM AvMC and the ISN produced a breakthrough in the generation of terahertz (THz) waves, which lie between microwaves and radio waves, and are key to improved technologies for secure wireless communications; high-resolution, short-range radar; and safe "see-through" imaging. More recently, the team demonstrated a THz laser that fits in a shoebox, runs at room temperature, and is tunable to different frequencies—like the dial of a radio—which is crucial to many applications.

CHALLENGE

THz waves only travel a short distance through air before being absorbed—from a few meters to hundreds of meters, depending upon the THz frequency—so they can be used for short-range communications or radar-like imaging that is invisible to eavesdroppers far away, and a tunable THz source can alter its range at will. Unlike radar, THz waves are small enough to resolve fine details, such as cracks in composite materials. Unlike microwave, infrared, or visible-light imaging, THz waves can "see through" plants, fabric, and other thin materials. Unlike x-rays, THz waves are safe for living things. But many practical applications are stymied by the difficulty of producing THz waves.

There have been many ways to generate THz waves, but they suffer from severe drawbacks, such as large size, ultra-cold cooling requirements, or a lack of tunability. One device, a THz laser, has been known since the 1970s but was relegated to the sidelines because it was thought to be bulky, inefficient, and non-tunable: a large tube filled with molecules that, in rare circumstances, could be caused to "rotate" and emit THz waves when illuminated by a specially tuned infrared laser. These THz molecular-gas lasers, however, turned out to have unexpected potential that could be unlocked by advances in theoretical understanding and infrared lasers.

"These gas lasers were for a long time seen as old technology, and people assumed these were huge, low-power, nontunable things, so they looked to other terahertz sources. Now we're saying they can be small, tunable, and much more efficient. You could fit this in your backpack, or in your vehicle for wireless communication or high-resolution imaging."

– Dr. Steven G. Johnson, MIT professor of applied mathematics and physics, and affiliated faculty member of the ISN (Chu, 2019)

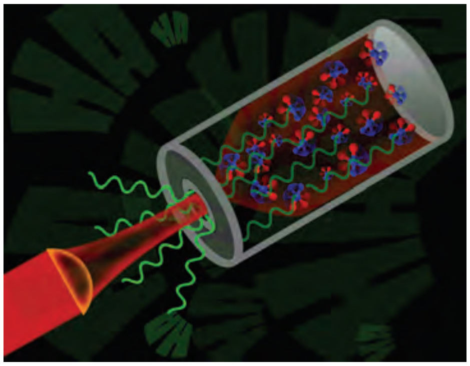


Figure 1: A new shoebox-sized laser produces THz waves (green squiggles) by using a special infrared laser (red) to rotate molecules of nitrous oxide, or laughing gas, packed in a pen-sized cavity (gray). Image adapted from Chu (2019).

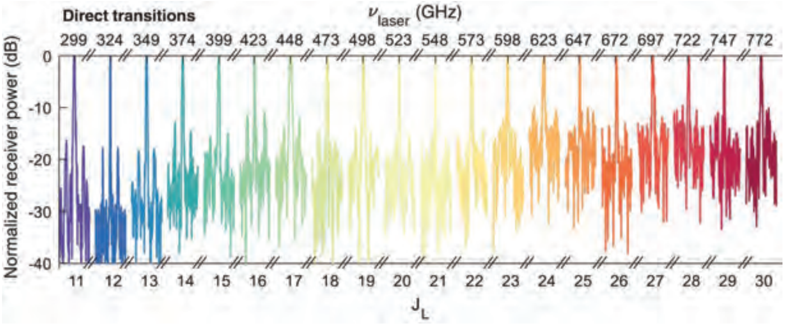


Figure 2: Emission spectra as the pump laser is tuned through different pumped transitions of nitrous oxide. Results show a fractional frequency tuning range of over 90%. Figure and caption adapted from Chevalier et al. (2019).

Several decades ago, Army scientist Dr. Henry Everitt of DEVCOM AvMC noticed an odd discrepancy in the behavior of THz molecular-gas lasers: the theoretical models predicted that they would stop working at high gas pressures (the molecules would bump into each other too frequently to emit THz waves), but his experiments showed that high pressures seemed to be no problem. For many years, this contradiction may have seemed to be only a puzzling footnote for an old technology. A few years ago, however, a collaboration between Dr. Everitt and Professors Steven Johnson, Marin Soljačić, and John Joannopoulos of MIT set out to develop a fully accurate theory for these THz gas lasers.

ACTION

Ongoing collaborations with scientists at DEVCOM AvMC emerged as a result of historical relationships established with MIT's ISN Director, an attribute of this long-term UARC program. An understanding of this THz research discovery will be shared across the Army modernization enterprise via a three-tiered approach whereby the ISN team will initially harness (1) the relevant ISN science and technology (S&T) partners followed by (2) the relevant AFC S&T ecosystem, and finally (3) the relevant partners across the DoD research community. By using this three-tiered approach, the ISN will identify transition interests and outline impact to Army modernization. Once the partners have been established for transition of the research discovery, the ISN will follow up with a series of relevant collaborative engagements that explore and exploit an iterative approach where basic research continues to inform transition to higher readiness levels.

RESULT

The first fruits of this collaboration, published in *Proceedings of the National Academy of Sciences* in 2018 (Wang et al., 2018), not only matched experiments perfectly, but offered a new life to this old technology by suggesting that THz gas lasers could be far more compact and far more efficient than had previously been suspected, in part by operating in the "contradictory" regime of higher pressures where the old theories had failed (Figure 1).

Moreover, the new theoretical model could be used to rapidly explore ways to improve THz wave generation by changing the type of gas molecule or the infrared energy source. In a collaboration with Professor Federico Capasso at Harvard University, the researchers

ARL Competencies:

- Sciences of Extreme Materials
- Photonics, Electronics, and Quantum Sciences
- Electromagnetic Spectrum Sciences

Results

- Led to co-publications between Army and academic researchers in the top journals *Science* and Proceedings of the *National Academy of Sciences*.
- Predicted and confirmed the viability of nitrous oxide for the production of THz laser light in QCLs.
- Demonstrated a compact, tunable, room-temperature THz laser.
- Enabled continued collaborative research and development between Army and academic scientists and engineers.

Anticipated Impact

The potential for room-temperature, portable, tunable THz lasers could lead to technologies such as advanced imaging, high-resolution short-range radar, and secure wireless communications for dismounted Soldiers as well as their platforms and vehicles.

discovered that a huge "menu" of molecules could potentially be made to lase using a compact type of infrared laser that did not exist in the 1970s, a quantum cascade laser (QCL). Because a single QCL is tunable to different "colors" of infrared, it could be tuned to cause almost any gas molecules to "rotate" and emit THz waves at any of its allowed frequencies. They identified a new gas—laughing gas (nitrous oxide)—that had never been used for THz lasing as a perfect fit for a readily available QCL. A laboratory experiment confirmed the theory: the new gas, and the new QCL, produced THz waves where the theory predicted, and could be tuned over a huge range of THz frequencies (Figure 2). Published in *Science* in 2019 (Chevalier et al., 2019), these results are pointing the way toward a new generation of THz applications.

WAY AHEAD

The ISN team will launch an Army Nanotechnology Seminar (ANTS) on this tunable THz wave generation advance that leverages affiliated university, Army, and industry partners that are aligned to support and potentially sponsor Army modernization. Next, the ISN will launch an ANTS on this THz laser discovery across the relevant Army S&T research development ecosystem with the goal of ultimately exploring opportunities to highlight this discovery across the DoD by engaging the Basic Research Office. As research and transition interests are identified, the ISN will work toward collaborative engagements, using the "teams of teams" approach, to operationalize this research discovery toward transformational overmatch capabilities.

This success was made possible by:

Mr. John R. McConville,
Physical Sciences Division

Dr. James Burgess,
Physical Sciences Division

Citations:

Chandler, D. L. "How to make ceramics that bend without breaking," *MIT News Office*. (2020).

Crystal, I. R., Lai, A. & Schuh, C. A. *J Am Ceram Soc*. **103**, 4678-4690 (2020).

Lai, A., Du, Z., Gan, C. L. & Schuh, C. A. *Science* **341**, 1505-1508 (2013).

Pang, E. L., McCandler, C. A. & Schuh, C. A. *Acta Mater.* **177**, 230-239 (2019).

SUCCESS STORY

Ductile Ceramics

An ARO-funded ISN team has made an important breakthrough by demonstrating a novel ceramic material that avoids catastrophic cracking during impact, providing a potential mechanism for mitigating the undesirable brittleness of ceramics. This gives promise for strong, ductile ceramics as a bulk material class that have a significantly enhanced mechanical energy absorption compared with existing armor ceramics.

CHALLENGE

Ceramics are extremely hard and strong materials. However, they are also brittle because their ionic/covalent bonds, once broken, do not readily reform like in metals. What is required to make ceramics ductile is a mechanism that allows atoms to reorganize under stress without breaking their bonds. Interestingly, zirconia ceramics have just such a mechanism, a martensitic phase transformation. This change in crystal structure accommodates deformation by skewing and tilting the bonds without breaking them. Unfortunately, this does not make zirconia ductile. In fact, samples of zirconia crumble to powder during a martensitic transformation such that when engineers wish to use zirconia for applications including medical implants and prostheses, they regularly add alloying elements to *suppress* the transformation.

These two factors may at first seem contradictory: martensitic transformations are key to allowing atoms to reorganize under stress without breaking bonds, but these same transformations inherently cause cracking. Since the first very reports of these phenomena in 1929, researchers have accepted as fact that zirconia "inevitably disintegrates by cracking" when it undergoes a martensitic transformation. However, closer examination of the scientific literature reveals that this "fact" is merely speculation; no one has demonstrated the chemical and mechanical origins of this cracking phenomenon and whether it can be avoided in zirconia.

The ISN team succeeded in overcoming this problem by realizing the issue is one of compatibility: as the material undergoes martensitic transformation, the transformed phase (which has a monoclinic crystal structure) must interface with untransformed regions (which have a tetragonal structure). The two structures must coexist, but unfortunately, they are quite geometrically dissimilar; because they do not match up perfectly, stresses build that initiate cracking across larger scales (Figure 3A). The trick is then to engineer special chemistries that have perfect compatibility between the transforming phases (Figure 3B).

ACTION

The ISN team will provide a shared understanding of this ductile ceramic research discovery across the Army modernization enterprise. The ISN will initially explore the relevant ISN S&T partners, followed by the relevant AFC S&T ecosystem, and finally across the relevant DoD S&T

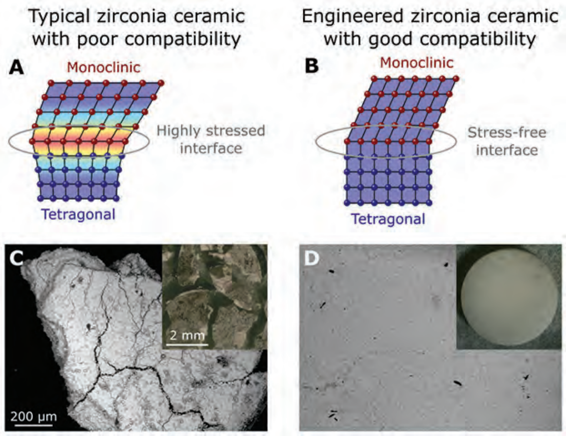


Figure 3: Interface between the tetragonal and monoclinic phases during martensitic transformation for (A) a typical zirconia ceramic with poor compatibility and (B) a highly engineered zirconia ceramic with good compatibility. Scanning electron (main) and optical (inset) micrographs of (C) a typical ZrO_2-$12CeO_2$ ceramic after one transformation cycle and (D) a carefully engineered ZrO_2-$13.5CeO_2$ ceramic after 10 transformation cycles. Image courtesy of Professor Christopher Schuh, MIT.

research community. By using this three-tiered approach, the ISN will identify interest in this discovery and its potential impact to Army modernization. Once the ISN has identified partners interested in transition of this discovery, the ISN will follow up with a series of relevant collaborative engagements that explore and exploit an iterative approach where basic science continues to inform transition plans coupled to the Army's modernization mission.

RESULT

The ISN team carefully engineered a cerium oxide (ceria)-doped zirconia material, ZrO_2-$13.5CeO_2$, with near-perfect compatibility in which no macroscopic cracking is visible after 10 thermal transformation cycles (Figure 3D). In stark contrast, a non-optimal ZrO_2-$12CeO_2$ composition fractures into many pieces after a single transformation cycle (Figure 3C). This illustrates that compatibility is indeed responsible for crack initiation and gives promise that the martensitic transformation in zirconia can accommodate deformation without cracking, thus giving rise to appreciable ductility by a transformation-induced plasticity (TRIP) effect as in steels.

While mechanical validation tests are currently ongoing, the exceptional strength of zirconia ceramics combined with this potential newfound ductility hints at tantalizingly large amounts of mechanical energy absorption, potentially increased by as much as 500% compared with existing armor ceramics (Figure 4). This would represent a paradigm shift in materials science to the point of confusing the meaning of the word “ceramic” and would also open up new application areas in engineering.

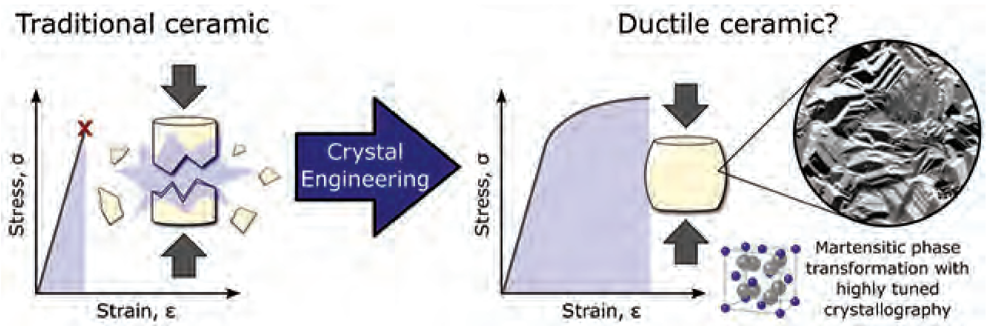


Figure 4: Schematic of a traditional ceramic exhibiting brittle fracture and a ductile ceramic undergoing martensitic transformation that absorbs a significantly larger amount of mechanical energy. Image courtesy of Professor Christopher Schuh, MIT.

WAY AHEAD

The ISN will first launch an ANTS on this ductile ceramic discovery. Focused on ISN S&T innovation, the ANTS will leverage affiliated university, Army, and industry partners that are aligned to support and potentially sponsor Army modernization. Next, the ISN will launch an ANTS on this ductile ceramic discovery across the relevant and targeted Army S&T research development ecosystem with the goal of expanding awareness across the DoD research enterprise by engaging the Basic Research Office. As transition partners are identified, the ISN will work toward collaborative engagements, using the “team of teams” approach, to operationalize this research discovery toward transformational overmatch capabilities.

ARL Competencies:

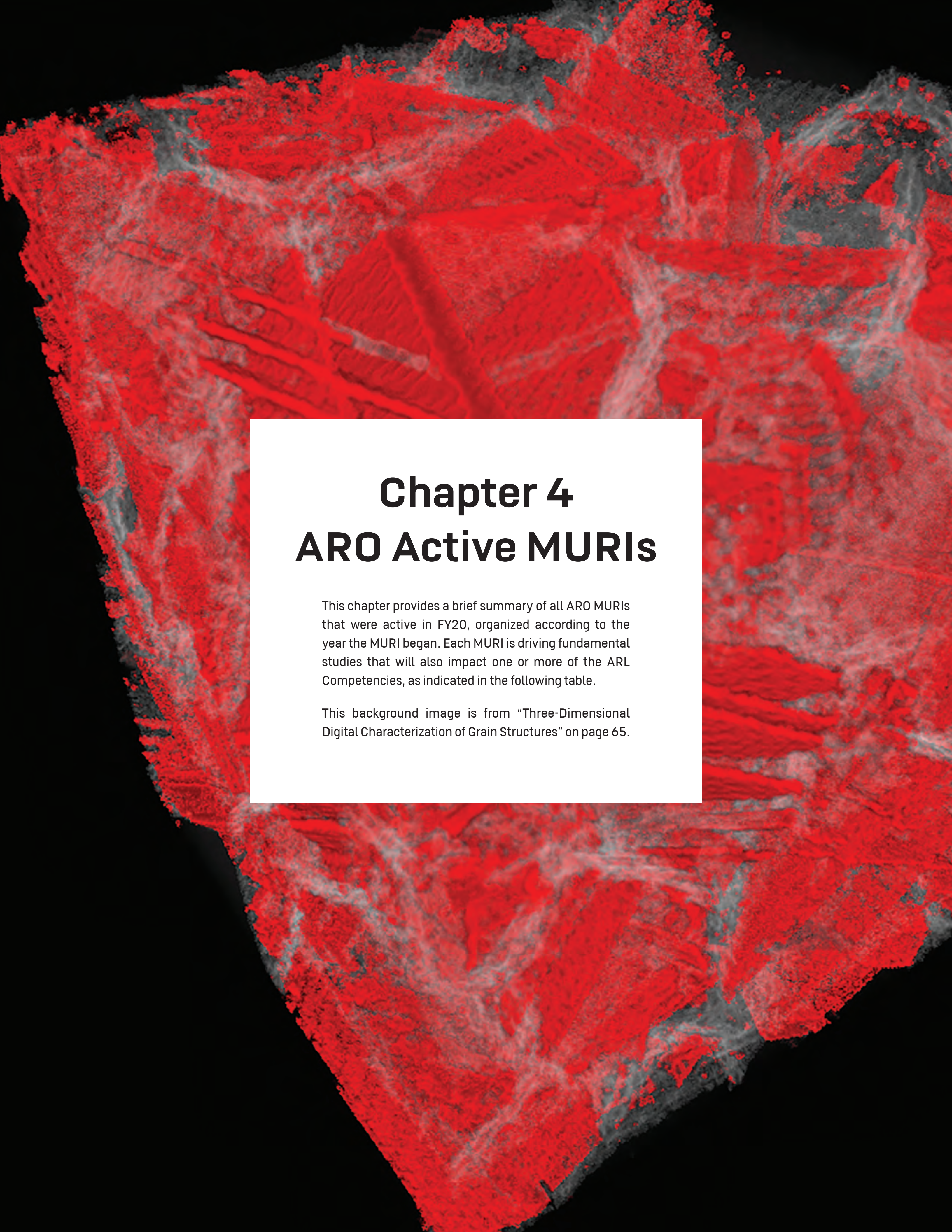
- Sciences of Extreme Materials
- Energy Sciences
- Mechanical Sciences

Results

- Published in leading journals including *Science* (Lai et al., 2013), *Acta Materialia* (Pang et al., 2019), and the *Journal of the American Ceramic Society* (Crystal et al., 2020).
- Initiated and continuing mechanical testing to validate experimental and computational results.

Anticipated Impact

The very existence of ductile ceramics could inspire entirely new areas of investigation in materials science. Practically manufactured ductile ceramics would likely lead to dramatic improvements in the effectiveness and robustness of a wide array of equipment—from tiny microactuators in electronic devices to, most notably, ballistic protective ensembles for the dismounted Soldier.



Chapter 4
ARO Active MURIs

This chapter provides a brief summary of all ARO MURIs that were active in FY20, organized according to the year the MURI began. Each MURI is driving fundamental studies that will also impact one or more of the ARL Competencies, as indicated in the following table.

This background image is from "Three-Dimensional Digital Characterization of Grain Structures" on page 65.

MURI Topic	Associated ARO PM/POC	Pg #	SEM	PE&QS	MIS	BBS	HCS	NS&CS	TE	WS	EMSS	ES	MS
Active MURIs that began in FY20													
Adaptive and Adversarial Machine Learning	Iyer	224					●	●					
Axion Electrodynamics beyond Maxwell's Equations	Qiu, Ulrich	224		●									
Engineering Endosymbionts to Produce Novel Functional Materials	Strand, Varanasi	224				●							
Information Exchange Network Dynamics	Cansever, Palazzolo	225						●					
Mathematical Intelligence: Machines with More Fundamental Capabilities	Myers, Gamble	225		●									
Quantum State Engineering for Enhanced Metrology	Baker, Qiu	225		●									
Solution Electrochemistry without Electrodes	Mantz	226										●	
Stimuli-Responsive Mechanical Metamaterials	Stanton, Poree	226	●										
Active MURIs that began in FY19													
How Sleep Clears Your Brain: Slow Waves, Glymphatic Waste Removal, and Synaptic Down-Selection	Munson, Gregory	227					●						
Formal Foundations of Algorithmic Matter and Emergent Computation	Stanton, Baker	227					●	●					
Networked Palynology Models of Pollen and Human Systems	Strand, Troyer	227				●	●						
Near-Field Radiative Heat Transfer and Energy Conversion in Nanogaps of Nano- and Meta-Structured Materials	Varanasi, Ulrich	229						●					
Investigating Energy Efficiency, Information Processing, and Control Architectures of Microbial Community Interaction Networks	Kokoska, Cansever	229						●					
Predicting and Controlling the Response of Particulate Systems through Grain-Scale Engineering	Myers, Barzyk	230	●					●					
Quantum State Control of Molecular Collision Dynamics	Parker, Baker	230		●							●		
Foundations of Decision-Making with Behavioral and Computational Constraints	Iyer, Palazzolo	230					●						
Active MURIs that began in FY18													
Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale	Varanasi, Govindan, Baker	231	●	●									
Multiscale Integration of Neural, Social, and Network Theory to Understand and Predict Transitions from Illness to Wellness	Palazzolo, Gregory	231					●						
Multiscale Network Games of Collusion and Competition	Iyer, Palazzolo	232					●	●					
New Materials from Dusty Plasmas	Bakas, Parker	232	●										
Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits	Gamble, Govindan, Stanton	233		●				●					
Science of Embodied Innovation, Learning and Control	Stanton	234					●						●
Stimuli-Responsive Control of Protein-Based Molecular Structure	McElhinny, Poree	234				●							
Toward a Multiscale Theory on Coupled Human Mobility and Environmental Change	Troyer, Cansever	235					●	●					
Active MURIs that began in FY17													
Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene	Baker, Ulrich, Varanasi	235	●	●									
Adaptive Self-Assembled Systems	Runnerstrom, Poree	235	●								●		●
Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems	Stanton, Munson	236											●
Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress	Gregory, Kokoska	236				●	●						
Realizing Cyber Inception: Toward a Science of Personalized Deception for Cyber Defense	Wang, Troyer	237						●					

MURI Topic	Associated ARO PM/POC	Pg #	SEM	PE&QS	MIS	BBS	HCS	NS&CS	TE	WS	EMSS	ES	MS
Room-Temperature Exciton-Polaritonics	Gerhold, Ulrich	237	●	●	●								
Semantic Information Pursuit for Multimodal Data Analysis	Krim	238						●					
Active MURIs that began in FY16													
Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy	Krim, Gregory	238				●	●	●					
Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning	Gregory, Pasour	239					●	●					
Discovering Hidden Phases with Electromagnetic Excitation	Ulrich, Varanasi	239	●										
Modular Quantum Systems	Govindan, Curcic (AFOSR)	239		●									
Multimodal Energy Flow at Atomically Engineered Interfaces	Anthenien, Mantz	240										●	
Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery	Poree, McElhinny	240				●							
Spin Textures and Dynamics Induced by Spin-Orbit Coupling	Qiu, Runnerstrom, Ulrich	242	●										
Socio-Cultural Attitudinal Networks	Iyer, Troyer	242					●						
Active MURIs that began in FY15													
Advanced 2D Organic Networks	Varanasi, Poree	243				●							
Emulating the Principles of Impulsive Biological Force Generation	Stanton, Kokoska	243				●							
Engineering Exotic States of Light with Superconducting Circuits	Govindan, Qiu	243		●									
Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications	Myers	244						●					
Imaging and Control of Biological Transduction using Nitrogen-Vacancy Diamond	Gregory, Baker	244				●							
Multiscale Responses in Organized Assemblies	Poree, Runnerstrom	245				●							
Network Science of Teams	Palazzolo	246						●					
Noncommutativity in Interdependent Multimodal Data Analysis	Krim, Govindan	246					●	●					
Active MURIs that began in FY14													
Attosecond Electron Dynamics	Parker, Ulrich	247		●							●		
Force-Activated Synthetic Biology	McElhinny, Cole	247				●							
Innovation in Prokaryotic Evolution	Strand, Myers	247				●							
Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials	Myers, Varanasi	248	●					●					
Multistep Catalysis	Mantz, Cole	248				●						●	
Ultra-Cold Molecular Ion Reactions	Baker, Parker	249		●									
Understanding the Skin Microbiome	Pasour, Kokoska	249				●	●						
Active MURIs that began in FY13													
Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation	Wang	250			●								
Artificial Cells for a Novel Synthetic Biology Chassis	McElhinny, Poree	250				●							
Nanoscale Control, Computing, and Communication Far-From-Equilibrium	Stanton	250			●								
Nonequilibrium Many-Body Dynamics	Baker, Ulrich	251		●									
Theory and Experiment of Co-Crystals: Principles, Synthesis, and Properties	Parker, Varanasi	251	●										

Overview of Active ARO MURIs

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in Chapter 2. These projects constitute a significant portion of the basic research programs managed by ARO; therefore, all of ARO's active MURIs are described in this section.

ACTIVE MURIS THAT BEGAN IN FY20

Adaptive and Adversarial Machine Learning

The goal of this MURI topic is to build adaptive machine learning (ML) systems that are capable of performing against corrupted training data, evasion attacks, and unexpected inputs. Achieving these goals requires mathematical and algorithmic development frameworks that are application- and implementation technique-independent. This framework should enable the development of robust and adaptive ML-based intelligent systems, with predictable properties and performance bounds that are capable of generalizing, reflecting, and reasoning in a contextual manner.

This MURI began in FY20 and was awarded to a team led by Professor Insup Lee, University of Pennsylvania. The objective of Professor Lee's effort is to develop the foundations for robust and adaptive learning based on childhood development. This will be achieved over three phases: (1) concept-based learning robust to adversarial examples, (2) adaptive learning in dynamic environments, and (3) verification and monitoring of learning. The approach will utilize concepts (e.g., prior models and shapes) inherent in the physical world , while simultaneously detecting and adapting to changes in the environment and concepts, such that robustness claims can be validated through a combination of offline verification and runtime monitoring. Evaluations of the techniques will be performed on an interactive robotic platform as a surrogate for future military applications involving cooperative robotic systems with learning in a battlefield environment.

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Purush Iyer, Computing Sciences Branch

Axion Electrodynamics beyond Maxwell's Equations

The goal of this MURI topic is to develop a new class of electric-field tunable axion device concepts such as electric-field switching of ferromagnets, voltage tunable magnetic inductors, filters, resonators, and non-reciprocal devices without current dissipation through a cohesive, multidisciplinary approach involving electronics, physics, and materials. This research will focus on the formation of pristine, atomic-level interfaces between (known) topological materials and non-topological materials; the physics of the intertwined electronic and magnetic phenomena amid electrical contacts and other media necessary in a real, non-idealized environment; and techniques for observing and exploiting the axion term for unique magnetoelectric effects in these heterostructures. In other words, the aim is to fundamentally understand axion electrodynamics in topological solid-state systems and demonstrate axion-based electric-field control of both electric and magnetic properties.

This MURI began in FY20 and was awarded to a team led by Professor Norman Peter Armitage, Johns Hopkins University. The objective of Professor Armitage's effort is to exploit the novel "axion" magnetoelectric response of topological materials—including magnetic topological insulators and Weyl semimetals—to generate new routes to couple electric and magnetic degrees of freedom in materials and devices. This will be achieved by combining state-of-the-art materials development, device fabrication, terahertz (THz) spectroscopy, analytical theory, electromagnetic (EM) modeling, nonlinear optics, and local probes of EM response to elucidate fundamental aspects of the axion response in topological systems. By focusing on axion electrodynamics, this research has the potential to unlock high-performance materials and devices capable of room-temperature operation of broad interest to both academic and DoD communities.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. Joe Qiu, Electronics Branch

Dr. Marc Ulrich, Physics Branch

Engineering Endosymbionts to Produce Novel Functional Materials

The goal of this MURI topic is to leverage recent advances in materials science and synthetic biology to develop a eukaryotic organism driven by a programmable prokaryotic organism and use the hybrid system to explore the creation of novel functional materials. Eukaryotic systems provide opportunities to realize more sophisticated products; however, these complex organisms present significant challenges to engineer and program. In a hybrid system, the best of both can be achieved: an engineered, prokaryotic endosymbiont controlling a eukaryotic host cell to produce materials

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Micheline Strand, Life Sciences Branch

Dr. Chakrapani Varanasi, Materials Science Branch

of interest. This project will explore the fundamental process of biosynthetic production of novel functional materials using a eukaryotic organism controlled by a more easily and rapidly engineered prokaryotic endosymbiont for rapid, flexible, modular control.

This MURI began in FY20 and was awarded to a team led by Professor Jeffrey Barrick, University of Texas at Austin. To address this challenge, Professor Barrick proposed to genetically engineer bacterial endosymbionts that live within the bodies of animals or plants into onboard control modules and molecular factories that enhance the production and properties of the biomaterials. Specifically, they will develop and demonstrate these transformational capabilities by engineering endosymbionts that enhance brochosomes—natural nanostructures with novel surface and optical properties that are produced by leafhopper insects. If successful, this research will address a longstanding, unsolved challenge in the ability to engineer hybrid systems whereby a prokaryotic endosymbiont controls a eukaryotic host cell to produce materials of interest, ultimately leading to a broad range of disruptive technologies having significant impact on DoD capabilities

Information Exchange Network Dynamics

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Drs. Derya Cansever and Edward Palazzolo, Network Sciences Branch

Recently observed differences between the propagation of legitimate and misleading news items in social media have made it necessary to revisit traditional models of information dynamics over networks. The goal of this MURI topic is to model the dynamics of cognitive processes over information networks for efficient information diffusion, controlling its veracity and forecasting potential cognitive outcomes of these dynamics. Achieving this goal requires leveraging recent advancements in experimental psychology, computer science, and information theory to enable understanding of information flow dynamics.

This MURI began in FY20 and was awarded to a team led by Professor Cedric Langbort, University of Illinois at Urbana-Champaign. To address this challenge, Professor Langbort will establish an understanding of the multimodal dynamics of information over networks by developing rigorous models of such multimodal information transmission that explicitly account for intentionality and capturing the effects of psycho-cognitive factors. More specifically, Professor Langbort proposes a multidisciplinary approach to address three interconnected research themes: (1) the development of models of intentional information transmission on networks, (2) their enrichment to incorporate behavioral elements such as lack of rationality and Bayesianity and the role of emotions, and (3) their validation in experiments and on preexisting datasets. This framework should enable the development of models that can determine how authentic information and misinformation are propagated differently, and devise ways to quantify misinformation spreading.

Mathematical Intelligence: Machines with More Fundamental Capabilities

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. Joseph Myers, Mathematical Sciences Branch

Dr. Sara Gamble, Physics Branch

Construction of error-free programs is empirically difficult, and error rates increase in line with their complexity. To overcome this challenge, experts are beginning to recognize that error-proof, machine-generated programming is mandatory when zero tolerance in execution is required. The goal of this MURI topic is to develop the new science of iteratively constructed logical deduction in the context of quantum field theories (non-relativistic, relativistic, and topological) for quantum information processing (QIP) and develop its basis as a foundation for certifiable automated reasoning. This will ultimately enable mathematically intelligent (MI) machines equipped with deduction, induction, and logical inference, capable of generating new insights that are certifiably correct.

This MURI began in FY20 and was awarded to a team led by Professor Arthur Jaffe, Harvard University. To address this challenge, Professor Jaffe proposes to investigate protocols, algorithms, complexity, error correction, and the certifiability of quantum processes using mathematical insights that combine picture calculus, quantum logic, and quantum field theory. By linking extremely abstract, theoretical ideas with practical laboratory implementation, the MURI team hopes to provide a rigorous theory for MI machines, ultimately enabling the construction of a quantum computer that can substantially improve present error correction codes.

Quantum State Engineering for Enhanced Metrology

Assured position, navigation, and timing is a high priority, especially for autonomous platforms. For platforms to maintain accurate knowledge of their position, orientation, and altitude during missions, the uncertainty errors accumulated over time have to be constrained by external aides. Quantum systems are a promising candidate to aid in minimizing uncertainty due to their demonstrated position. Two important questions about quantum sensors remain: (1) Can special quantum states be realized that push the performance of these sensors to the fundamental limit? (2) Can these systems be engineered such that their exquisite sensitivity is constrained to what one intends to measure? The goal of this MURI topic is to investigate these knowledge gaps and develop methods that explore quantum correlations and special states to enhance metrology, improve sensitivity, achieve fundamental uncertainty limits in different ways, and integrate these states with thermal reservoirs and strong system design to mitigate decoherence.

This MURI began in FY20 and was awarded to a team led by Professor Monika Schleier-Smith, Stanford University. To address this challenge, Professor Schleier-Smith proposes to develop protocols for generating metrologically powerful entangled states that are robust to develop real-world noise and realistic experimental imperfections to explore how resilient entanglement is in the real world. By comparing idealized experiments to disordered solid-state platforms, the MURI team will develop the tools necessary to transfer techniques from well-controlled academic labs to the field. The techniques will enable next-generation atomic clocks with world-leading, short-term stability and robustness to noise. Ultimately, this effort will result in a clear assessment of when entanglement provides a practical win for real-world sensors, and a roadmap of algorithms and platforms necessary to make such sensors a reality.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. Paul Baker, Physics Branch

Dr. Joe Qiu, Electronics Branch

Solution Electrochemistry without Electrodes

Traditionally, electrochemistry is focused on a system where electron transfer occurs at an electrode surface. In these systems, the electroactive species interacts with the electrode and this interaction has an effect on electron transfer. Recent advancements in the surface plasmon decay of metallic nanoparticles coupled with light and atmospheric plasmas have been used to generate electrons, indicating that non-electrode electrochemistry is feasible. However, to date, very little research has been dedicated to using surface plasmon-based systems to drive solution electrochemical reactions. The goal of this MURI topic is to explore and understand the electrochemistry between electrons that have been generated by methods such as atmospheric plasma, surface plasmon, or pulsed radiolysis and solution species. This effort is focused not only on controlling the generation of electrons, but also the characterization of their energies and lifetimes including electron penetration and diffusion to solution species, as well as novel solution electrochemistry and electrosynthesis.

This MURI began in FY20 and was awarded to a team led by Professor Peter Bruggeman, University of Minnesota, Twin Cities. To address this challenge, Professor Bruggeman proposes to investigate foundational scientific questions addressing plasma-induced species in solutions and their role in chemical transformation. This will be achieved by exploiting recent advancements in pulsed power and radio frequency plasmas to enable unprecedented controllable injection of electrons into solution on nanosecond timescales commensurate with the typical lifetime of reactive intermediates in solution. The resulting improved control of electron and ion fluxes and energies incident into the solution will enable synthesis of nanoparticles and polymers with desired but previously uncontrollable or unattainable properties.

ARL Competencies:

Energy Sciences

MURI Author(s) and Manager(s):

Dr. Robert Mantz, Chemical Sciences Branch

Stimuli-Responsive Mechanical Metamaterials

Metamaterials research has categorically demonstrated the potential for microarchitected materials to surpass the intrinsic properties and functionality of natural and conventional materials. Notable advances in chemical triggering mechanisms and nanomaterial assembly has opened doors to fabricating stimuli-responsive mechanical metamaterials with unprecedented architectural control. However, realizing the utmost potential for rationally designed active metamaterials requires research on the role of interfacial phases as well as pathways for integrating modern understanding of metamaterial wave dynamics and topological mechanics. To fully realize the potential of responsive metamaterials, this MURI is focused on creating stimuli-responsive mechanical metamaterials with precise nanoscale interparticle, interfacial, and functional control.

This MURI began in FY20 and was awarded to a team led by Professor Nicholas Boechler, University of California, San Diego. To address this challenge, Professor Boechler proposes to investigate the fundamental structure–activity relationships that govern the interplay of metamaterial mechanics and changes in the properties of the primary constituent material. More specifically, the MURI team will target challenges at the intersection of metamaterials and stimuli-responsive materials including the slow active response in metamaterials with stimuli-responsive constituent materials, the one-way response of stimuli-responsive constituent materials, and the application of these topological

ARL Competencies:

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. Samuel Stanton, Mechanical Sciences Branch

Dr. Dawanne Poree, Chemical Sciences Branch mechanics at micro- to sub-nanoscales. This will be achieved by pursuing a series of experiments where the responsive chemistries employed act as chemical triggers that will initiate chemical signals in the form of electrons and protons, which will induce a material response in the form of change in modulus, shape, or addition/removal of material. These advances will lead to new types of metamaterials that have unprecedented capabilities for energetic transformation and wave control, ultimately informing the design of DoD-relevant stimuli responsive material systems.

ACTIVE MURIS THAT BEGAN IN FY19

How Sleep Clears Your Brain: Slow Waves, Glymphatic Waste Removal, and Synaptic Down-Selection

ARL Competencies:

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Matthew Munson, Mechanical Sciences Branch

Dr. Frederick Gregory, Life Sciences Branch

This MURI began in FY19 and was awarded to a team led by Professor Maiken Nedergaard, University of Rochester. The goal of this MURI topic is to develop a framework describing the interplay of small-scale multiphase flows with biochemical and neurophysiological processes to quantitatively characterize glymphatic clearance dynamics and regulation mechanisms. This framework should account for disparate scales in both length and time, such that the reciprocal impact of cellular-scale processes on system-level regulatory phenomena (e.g., sleep) can be described and predicted. Additionally, strategies for exogenous manipulation of waste clearance to assess the impact on neurocognitive performance (e.g., alertness, learning, and memorization) should be explored.

The objective of this proposal is to examine the hypothesis that slow waves and the underlying ON/OFF bistability of thalamic and cortical neurons not only drive synaptic down-selection but also promote glymphatic flow by the coordinated movement of ions (Na^+, K^+, Cl^-) across the neuronal membranes during UP and DOWN states, which move from front to back and are detected as slow wave activity (SWA). The proposal seeks to (1) demonstrate at the highest possible temporal and spatial resolution that glymphatic function, synaptic down-selection, and slow waves are linked; (2) characterize the underlying mechano-electro-chemical mechanisms that link these processes; and (3) determine whether facilitating these processes can increase the beneficial effects of sleep and improve neurocognitive performance.

For more information on this effort, check out the ARO in the News feature on the next page!

Formal Foundations of Algorithmic Matter and Emergent Computation

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Samuel Stanton, Mechanical Sciences Branch

Dr. Paul Baker, Physics Branch

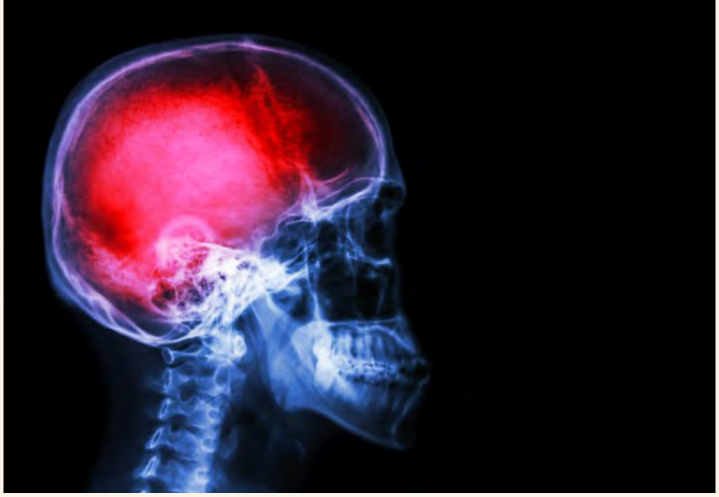
This MURI began in FY19 and was awarded to a team led by Professor Dana Randall, Georgia Institute of Technology. This MURI topic has two concurrent objectives: (1) synthesize advances in nonequilibrium information physics with natural algorithms and decentralized control to identify principles governing how local algorithms, negative and positive feedback, fluctuation amplification, and the topology of information flow lead to unanticipated patterns and information processing in natural self-organizing systems; and (2) develop novel experimental systems to challenge and extend the theory and additionally achieve directed self-organization. That is, demonstrate guided discovery of optimal information processing patterns or reconfigurable robustness to harmful emergent phenomena (e.g., failure modes) by actively biasing the environment or manipulating the self-organization information-energy landscape.

This MURI focuses on systems that define algorithmic (active) matter: ensembles of particles that interact locally leveraging their physical characteristics and their interaction with the environment, using limited computational resources, bounded communication, and bounded memory to achieve complex tasks.

The specific objectives of the proposed effort are to (1) predict physical and computational requirements for emergent computation, (2) determine what nonequilibrium characteristics cause these systems to evolve toward the desired emergent behavior, and (3) design efficient collective computational systems to achieve specific task-oriented goals.

Networked Palynology Models of Pollen and Human Systems

This MURI began in FY19 and was awarded to a team led by Professor Anthony Grubesic, Arizona State University. The goal of this MURI topic is to develop both mathematical and computational modeling



ARO IN THE NEWS

Army research may improve stroke, TBI treatment

By U.S. Army CCDC Army Research Laboratory Public Affairs
February 4, 2020

New Army research provides a better understanding of the swelling that occurs in the brain during a stroke, which could contribute to new treatment strategies for stroke patients and have potential implications for traumatic brain injuries.

Cerebral edema, swelling that occurs in the brain, is a severe and potentially fatal complication for stroke victims. Research, funded in part by the Army Research Office and conducted at The University of Rochester Medical Center, shows for the first time that the glymphatic system -- normally associated with the beneficial task of waste removal -- goes awry during a stroke and floods the brain, promoting edema and drowning brain cells.

The research, conducted with mice, appears in the journal Science.

> **"These findings show that the glymphatic system plays a central role in driving the acute tissue swelling in the brain after a stroke," said Maiken Nedergaard, M.D., D.M.Sc., co-director of the University of Rochester Medical Center Center for Translational Neuromedicine and senior author of the article. "Understanding this dynamic -- which is propelled by storms of electrical activity in the brain -- point the way to potential new strategies that could improve stroke outcomes."**

The glymphatic system, first discovered by the Nedergaard lab in 2012, consists of a network that piggybacks on the brain's blood circulation system and is comprised of layers of plumbing, with the inner blood vessel encased by a 'tube' that transports cerebrospinal fluid. The system pumps the fluid through brain tissue primarily during sleep, washing away toxic proteins and other waste.

Before the findings of the new study, scientists assumed that the source of brain swelling was exclusively the result of fluid from blood.

"Our hope is that this new finding will lead to novel interventions to reduce the severity of ischemic events, as well as other brain injuries to which Soldiers may be exposed," said Matthew Munson, Ph.D., program manager, fluid dynamics, ARO, an element of the U.S. Army Combat Capabilities Development Command's Army Research Laboratory. "What's equally exciting is that this new finding was not part of the original research proposal. That is the power of basic science research and working across disciplines. Scientists 'follow their nose' where the data and their hypotheses lead them -- often to important unanticipated applications."

AN ELECTRICAL WAVE, THEN THE FLOOD

Ischemic stroke, the most common form of stroke, occurs when a vessel in the brain is blocked. This blockage denies the nutrients and oxygen cells need to function, which results in their rapid depolarization. As the cells release energy and fire, they trigger neighboring cells, creating a domino effect that results in an electrical wave that expands outward from the site of the stroke, called spreading depolarization.

During the spreading depolarization, vast amounts of potassium and neurotransmitters released by neurons into the brain cause the smooth muscle cells that line the walls of blood vessels to seize up and contract, cutting off blood flow in a process known as spreading ischemia. Cerebrospinal Fluid then flows into the ensuing vacuum, inundating brain tissue and causing edema. The already vulnerable brain cells in the path of the flood essentially drown in fluid and the brain begins to swell. These depolarization waves can continue in the brain for days and even weeks after the stroke, compounding the damage.

> **"When you force every single cell, which is essentially a battery, to release its charge it represents the single largest disruption of brain function you can achieve -- you basically discharge the entire brain surface in one fell swoop," said Humberto Mestre, M.D., a Ph.D. student in the Nedergaard lab and lead author of the study. "The double hit of the spreading depolarization and the ischemia makes the blood vessels cramp, resulting in a level of constriction that is completely abnormal and creating conditions for CSF to rapidly flow into the brain."**

The study correlated the brain regions in mice vulnerable to the fluid propelled by the glymphatic system with edema found in the brains of humans who had sustained an ischemic stroke.

POINTING THE WAY TO NEW STROKE THERAPIES

The findings suggest potential new treatment strategies that, used in combination with existing therapies, focus on restoring blood flow to the brain quickly after a stroke. The study could also have implications for brain swelling observed in other conditions such as subarachnoid hemorrhage and traumatic brain injury.

Approaches that block specific receptors on nerve cells could inhibit or slow the cycle of spreading depolarization. Additionally, a water channel called aquaporin-4 on astrocytes -- an important support cell in the brain -- regulates the flow of the fluid. When the research team conducted the stroke experiments in mice genetically modified to lack aquaporin-4, the fluid flow into the brain slowed significantly.

Aquaporin-4 inhibitors currently under development as a potential treatment for cardiac arrest and other diseases could eventually be candidates to treat stroke.

In additional to the Army Research Office, the research was supported with funding from National Institute of Neurological Disorders and Stroke, the National Institute of Aging, Fondation Leducq Transatlantic Networks of Excellence Program, the Novo Nordisk and Lundbeck Foundations, and E.U. Horizon 2020.

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Drs. Micheline Strand and Lisa Troyer, Life Sciences Branch

approaches that will transform our ability to model and predict the distribution of plant species and pollen across space and time. These advances will create a completely new capability: the ability to accurately model and predict species distribution, with human effects fully integrated.

The objective of the proposed research is for biologists, geographic information scientists, and social scientists to work together to develop, instantiate, and validate networked palynology models of pollen and human systems to exploit the geographic information embedded in pollen for forensic purposes. The investigators will develop an open-source geocomputational toolbox based on next-generation species distribution models, which will locate forensic and other samples that are geographically indeterminate based on inputs from pollen DNA metabarcoding. They will extend the use of standard DNA metabarcoding for identifying pollen samples, with a particular focus on quantification not just presence/absence. They will develop a rapid-deployment sampling framework for capturing airborne pollen and also use pollinators as environmental samplers, particularly for low-abundance pollen. They will develop quantitative validation methods for determining the accuracy, precision, and uncertainty of developed species distribution models and geocomputational models. Pollen samples, including forensic, airborne, and pollinator from a variety of geographically known sources, will be used. Finally, they will leverage their strengths in social network models and applications as well as mathematical optimization to enhance the inference and predictive elements of the proposed work to extend the model from single-location attribution to multi-location attribution.

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Chakrapani Varanasi, Materials Science Branch

Dr. Marc Ulrich, Physics Branch

Near-Field Radiative Heat Transfer and Energy Conversion in Nanogaps of Nano- and Meta-Structured Materials

This MURI began in FY19 and was awarded to a team led by Professor Sangi Reddy, University of Michigan. The goal of this MURI topic is to determine the mechanisms responsible for radiative heat transfer between the surfaces of nanomaterials and between metasurfaces separated by nanoscale gap sizes in near-field and extreme near-field regimes and discover possible novel phenomena enabled by novel nano-materials/structures in these regimes.

The objective of this proposal is to understand the fundamental principles of novel near-field radiative heat transfer (NFRHT) phenomena such as NFRHT in ångström-sized gaps (i.e., extreme NFRHT [eNFRHT]) and NFRHT between non-reciprocal, nanostructured 2D and phase-change materials, as well as novel near-field energy conversion phenomena. The technical approach is based on a solid theoretical foundation and backed by sufficient computational studies. The proposed experimental platform to explore various NFRHT phenomena is proven and feasible. There is a series of novel materials and designs planned including dynamic control of NFRHT with phase-change materials, gate-tunable NFRHT, metasurfaces for spectral control, and eNFRHT in nanogaps.

One novel and very exciting concept proposed by the team includes a persistent thermal current akin to the quantum Hall effect (QHE). The team has proposed a clever approach that should allow such counterintuitive persistent currents. Another strong component of the proposal is the incorporation of near-field energy conversion. By including thermophotovoltaics into the NFRHT concepts, the team aims to advance the fundamental science and engineering of this aspect of energy conversion.

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Robert Kokoska, Life Sciences Branch

Dr. Derya Cansever, Network Sciences Branch

Investigating Energy Efficiency, Information Processing, and Control Architectures of Microbial Community Interaction Networks

This MURI began in FY19 and was awarded to a team led by Professor James Boedicker, University of Southern California. The goal of this MURI topic is to develop and validate a computational understanding of how information transfer arises within system architectures in biological communities across nature's evolutionary space and identify universal scaling principles from those models that are common to these various community structures.

The objective of this MURI is to develop a comprehensive model of biological communication by integrating four interconnected aspects of information flow within networks that span multiple scales of biological organization: (1) the connection between single-cell heterogeneity and decision-making within populations, (2) the optimization of information flow over multiple length and time scales, (3) the robustness and controllability of complex dynamic systems, and (4) information exchange between multiple layers of biological organization and the scaling of communication architectures for unicellular organisms to networks of multicellular organisms.

Predicting and Controlling the Response of Particulate Systems through Grain-Scale Engineering

This MURI began in FY19 and was awarded to a team led by Professor Jose Andrade, California Institute of Technology. The goal of this MURI topic is to enable efficient and accurate simulation of granular systems in nature and link particulate behavior across scales to enable efficient control algorithms within these systems.

This proposal will establish a framework to predict the continuum behavior of particulate systems by understanding and engineering a set of grain-scale features, termed here dynamic network attributes. The proposed work will develop the hypothesis that continuum behavior is encoded at the scale where neighboring grains interact. This proposal takes a radically different approach from the state of the art by directly embracing the interconnection between the different spatial scales that interact in granular assemblies: grain, meso, and continuum scale. The MURI builds on multiple areas of knowledge including physics, mechanics, mathematics, and engineering. The multidisciplinary approach affords the proposal the great advantage of transforming the state of knowledge across disciplinary boundaries that, historically, have been silos of specialized knowledge. Likewise, it will use and develop the most advanced experimental techniques (e.g., x-ray, force measurements) and connect these to continuum building blocks such as effective stress and constitutive models. Each of the areas is led by world experts in the field. The project will also strike a balance among theoretical, experimental, and computational approaches covering more than 6 orders of magnitude.

ARL Competencies:

Network Science and Computational Sciences

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. Joseph Myers, Mathematical Sciences Branch

Dr. Julia Barzyk, Mechanical Sciences Branch

Quantum State Control of Molecular Collision Dynamics

This MURI began in FY19 and was awarded to a team led by Professor Arthur Suits, University of Missouri. The goal of this MURI topic is to prepare high densities of molecular species in selected vibrational, rotational, and angular momentum states and study their reactive and nonreactive scattering dynamics in cold molecular beams.

The objective of the proposed research is the preparation of high densities of quantum states in molecular beams using techniques of quantum control and the study of quantum molecular collision dynamics as a function of the initially prepared state. Quantum degrees of freedom to be controlled in state preparation include translational, rotational, vibrational, and electronic. The research approach will draw on experimental and theoretical developments pioneered by the team members who hail from both chemistry and physics departments. Specifically, the team will pursue new coherent state preparation methods using lasers and molecular beams to generate molecules in perfectly defined vibrationally excited initial states, then use these uniquely prepared reactants in novel scattering experiments. At the same time, state-of-the-art theoretical investigations of the interatomic forces and the quantum scattering processes will be used to understand, model, and interpret the experimental results. The effort will probe new aspects of molecular interactions and chemical reactivity under highly controlled conditions. The following thrust areas in the proposal relate to the various approaches to be taken: Stark-induced Adiabatic Raman Passage and Related Methods, Stimulated Emission Pumping, Photo Association and Direct Cooling, Machine Learning and Electronic Structure Theory, and Collision Dynamics.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

MURI Author(s) and Manager(s):

Dr. James Parker, Chemical Sciences Branch

Dr. Paul Baker, Physics Branch

Foundations of Decision-Making with Behavioral and Computational Constraints

This MURI began in FY19 and was awarded to a team led by Professor Ali Jadbabaie-Moghadam, Massachusetts Institute of Technology (MIT). The goal of this MURI topic is to create predictive models of information flow through (human) networks (with biases) through generalization of noncommutative probability theory and information theory.

The approach proposed is to interpret bounded rationality as the result of limited resources and ambiguity in language, among humans, rather than as one necessitating complicated mathematics to interpret humans. The team will use inspiration from successful use of resource-boundedness in Turing machines to describe both structural and computational complexity, and derive a family of models between bounded and unbounded rationality. In doing so, the team will integrate both cognitive science and computational social science perspectives to address problems in decision theory. Experiments by the cognitive scientists on the team would be used to validate the mathematical theories proposed.

ARL Competencies:

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Purush Iyer, Computing Sciences Branch

Dr. Edward Palazzolo, Network Sciences Branch

The proposed approach is to approximate non-Bayesian reasoning using a form of Bayesian reasoning under structural and resource constraints, an idea borrowed from complexity theory in theoretical computer science, starting with current work on explaining a DeGroot-style reasoning (a nonlinear, non-Bayesian) system as Bayesian reasoning under certain resource constraints. The proposed work will make use of ideas from nonlinear utility, sampling, planning, distributed learning, computation complexity, and is divided into three thrusts: (1) developing foundational models of individual decision-making under computational and cognitive constraints, aiming to build from principled and well-documented behavioral biases and deviations from rationality; (2) developing a theory of group decision-making, along with a framework for analyzing decision-making models; and (3) executing computational and online experiments to test the theories from thrusts 1 and 2.

ACTIVE MURIS THAT BEGAN IN FY18

Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale

ARL Competencies:

Sciences of Extreme Materials

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. Chakrapani Varanasi, Materials Science Branch

Drs. T. R. Govindan and Paul Baker, Physics Branch

This MURI began in FY18 and was awarded to a team led by Professor Dirk Englund, MIT. The goal of this MURI is to develop novel solid-state host materials with unique color centers exhibiting extraordinary quantum properties at room temperature (low spectral diffusion, long coherence times, etc.), determine the composition processing defect property relationships governing these unique properties, and explore new concepts in quantum science (e.g., multi-photon states) enabled by these new materials. In the long term, discoveries from this MURI may lead to several key quantum technologies, including single- and entangled-photon emission, quantum sensors, and quantum memories.

Significant progress has been achieved in understanding and utilizing the quantum properties of optically addressable nitrogen-vacancy (N-V) color centers in diamond for quantum sensing and communication; however, further advances have been severely limited by difficulties in achieving exact placement of N-V centers, light collection due to the high refractive index of diamond, large-scale integration, and low qubit yield. Superior solid-state host materials include 3D wide bandgap semiconductors (e.g., silicon carbide [SiC], zinc oxide [ZnO], etc.) and recently discovered atomically thin 2D van der Waals materials (e.g., hexagonal boron nitride [h-BN], tungsten diselenide [WSe2]). With varieties of optically addressable color centers (far beyond N-V centers) are very attractive alternatives to advance this science. In addition, these alternative materials could also offer new opportunities not yet accessible such as multi-photon states, interactions between color centers, nonlinear quantum optics, etc.

The MURI team will employ extensive expertise in ab-initio calculations, 2D materials fabrication and manipulation, 3D atomic imaging, and quantum spectroscopy to enable an integrated feedback loop of ab-initio design, fabrication, imaging, and characterization of quantum materials at the atomic scale. The team is also developing first-of-a-kind tools for reconstructing 3D and 2D materials fully at the atomic scale, and developing revolutionary tools for nanometer-scale and even atomic-scale fabrication of quantum emitter systems. Lastly, the team will develop revolutionary chip-integrated quantum devices, including for quantum error corrected memories, entanglement-assisted sensors, and super-radiance/sub-radiance control.

Multiscale Integration of Neural, Social, and Network Theory to Understand and Predict Transitions from Illness to Wellness

ARL Competencies:

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Edward Palazzolo, Network Sciences Branch

Dr. Frederick Gregory, Life Sciences Branch

This MURI began in FY18 and was awarded to a team led by Professor Emily Falk, University of Pennsylvania. The goal of this MURI is to identify and model the coevolutionary dynamics of neural, cognitive, and social networks as people transition between illness and wellness while engaged in rapid integration treatment modalities. In the long term, discoveries from this MURI may reveal the neural and social network mechanisms involved in the transition from illness to wellness, and identify specific mechanisms that can be efficiently targeted to identify and alter the trajectory of adverse behavior (e.g., substance abuse) that may impact an individual's or team's safety.

Network science advances in social network analytics and brain connectomics allow for greater understanding of network effects impacting mood and brain states. New mathematical and statistical models allow for unprecedented analysis of information dissemination and decision-making. Recent research shows the impact of complex interactions between people's behavior and the route of messages through their social networks with respect to smoking behaviors, obesity, and the spread of happiness. Likewise, studies exploring mindfulness show measurable impact on human behavior as well as communication patterns between several brain regions. With greater understanding of the impact of social network connections (such as family, friends, healthcare teams, and weak ties) on the behavior of individuals embedded in society, attention must be turned to developing a foundational science to quantify how individuals' bodies and minds are impacted by such social forces and vice versa.

Neuroscience advances in mapping human neural activity can now be combined with social and cognitive network research to understand how people are connected to others and the causal impact of messages from their social network on changes in their brain states. These advances are relevant to understanding individuals who suffer from a variety of conditions such as post-traumatic stress disorder (PTSD), depression, anxiety disorder, substance abuse/addiction, and fibromyalgia/chronic pain.

This project is developing a multiscale model of intra-individual (i.e., neural, cognitive, physiological) and extra-individual (i.e., social) processes using an experimental manipulation of mindfulness and hypnosis, and characterizes interactions between baseline social network resources and regulatory strategy on dynamic neural responses and controllability, and downstream cognitive, physiological, and behavioral outcomes. The team will also experimentally perturb social network structure to further validate and refine the model.

Multiscale Network Games of Collusion and Competition

This MURI began in FY18 and was awarded to a team led by Professor Mingyan Liu, University of Michigan. The goal of this MURI is to create a new compositional game theory framework for characterizing the dynamics of interaction between multi-genre networks that could potentially share members or have weak links. In the long term, discoveries from this MURI may lead to new methods to drive improved agility of DoD responses to a broad spectrum of real-world security risks, as risk heterogeneity is fundamentally tied to scale, spanning nation states and lone-wolf actors.

Advances in scalable algorithmic techniques have made game theory a practical tool in a number of security-related applications, especially in the context of adversaries and defenders modeled in a two-party game. In practical situations, however, there are social networks that underlie adversarial and defender groups, respectively, with potential weak links between members of opposing groups that are effectively used by both groups to infiltrate the other. Examples include the use of double agents in infiltrating gangs and non-state adversarial groups, targeting of weak members in herd of deer, and targeting of specific T-cells in tumors. The dynamics of networks on networks is an ill-understood problem, especially the use of weak links in strategic decisions. Furthermore, there are situations, such as in modeling adversarial groups embedded in an ally's host population, where the need to consider multi-party interactions at multiple scales becomes important. The host population while agreeing that the adversarial group is a threat to society is nevertheless sympathetic to the issues raised by the adversarial group. In such cases, an intuitive strategy might be to influence the sentiment of the masses while targeting individuals in the adversarial group with each success (or failure) of the defender, resulting in a weakening (or emboldening, respectively) of the adversarial group. A meaningful mathematical analysis would require a multiscale framework in which both the coarse-grained model (e.g., of the host population) and the fine-grained model (of the social network of adversaries) need to be reasoned about.

This project is addressing the notion of abstraction and refinement in the context of network games, a class of n-party games where the network structure among the participants plays a role in distributed strategies. The research is addressing inference and decision/control problems. The inference problems involve studies to identify a multiscale network structure from potentially incomplete observational data. The decision/control problems involve the design of effective control and intervention schemes at appropriate levels of the network in order to induce desirable individual as well as group behaviors.

ARL Competencies:

- Humans in Complex Systems
- Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Purush Iyer, Computing Sciences Branch

Dr. Edward Palazzolo, Network Sciences Branch

New Materials from Dusty Plasmas

This MURI began in FY18 and was awarded to a team led by Professor Uwe Kortshagen, University of Minnesota. The goal of this MURI is to elucidate and control plasma-material dynamics, concomitant with complementary novel consolidation strategies, to realize robust plasma-based

ARL Competencies:

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. Michael Bakas, Materials Science Branch

Dr. James Parker, Chemical Sciences Branch

synthesis of 3D free-standing macrostructures via controlled consolidation of a wide range of discrete dust particles. In the long term, discoveries from this MURI may lead to directed-energy applications and advanced metamaterials with responsive properties for sensing and protection.

Research over the last decade has demonstrated that plasmas offer a means of levitating and manipulating "dust" particles of any material into controlled organized structures (i.e., plasma "crystals") of up to tens of centimeters in size. Concurrently, magnetic plasma confinement chambers have shown abundant material accumulation and fast convective transport. This accumulation motivated advances in the understanding of plasma magnetohydrodynamics (MHD), in addition to accurate predictions of the spatial distribution of dust particles and their individual trajectories. These efforts provide the scientific basis to realize a new paradigm in custom material design: consolidation of 3D free-standing materials and structures from plasma "dust." As plasmas can be created from any element and any material can be arranged in a plasma crystal, novel chemical reactions can be identified incorporating the free electrons, ions, and neutrals of a plasma to enhance manipulation and consolidation.

The MURI team is pursuing these studies at four highly interconnected levels: synthesis of particle building blocks, consolidation of these building blocks into macroscopic materials, materials design and characterization, and overarching theory and simulation. At the synthetic level, research will focus on advancing the state of the art from the current level of producing particles with homogeneous chemical composition of well-known phases to particle materials with nonequilibrium phases and composed of heterostructures. At the plasma consolidation level, the team will focus on controlling agglomeration to assemble macroscopic materials and elucidating the new physical mechanisms that will be encountered when incorporating dust crystals into free-standing macroscopic materials. Materials characterization will focus on establishing processing–structure–property relationships and demonstrating new material design paradigms on test-bed photonic materials.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Drs. Sara Gamble and T. R. Govindan, Physics Branch

Dr. Samuel Stanton, Mechanical Sciences Branch

Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits

This MURI began in FY18 and was awarded to a team led by Professor Kenneth Brown, Duke University. The goals of this MURI are to discover and devise approaches in which new, sensing, "spectator" qubits enable real-time characterization and verification of classical environmental factors, which, when uncontrolled, decohere qubits, and develop optimal statistics and computer science based techniques for collecting and analyzing spectator qubit data. In the long term, discoveries from this MURI have broad applicability to all areas of quantum information science, which is of great interest to DoD for potential needs in logistics, optimization, and the quantum simulation of materials.

A multidisciplinary focus on qubit physics, materials, fabrication, and operation has resulted in orders of magnitude improvements in key qubit performance metrics. Concurrently, new computer science, statistics, and engineering based control techniques such as Hamiltonian parameter estimation, machine learning, and robust control of classical fields have enabled novel quantum control and feedback approaches. The time is opportune to expand the necessary multidisciplinary approach to a systems view of a complex quantum system operating in a classical environment by integrating the new control, feedback, and sensing concepts with qubit physics to provide the next order of magnitude improvement in qubit performance. Currently, in state of the art, the qubit classical environment is rarely fully characterized during qubit operations in a qubit-focused, rather than an integrated system-focused, experiment.

Qubits often provide the most sensitive and precise measurements of the variability and noise in the classical environment in which they operate and, consequently, have recently been developed as high-performance sensing and metrology tools. Recent quantum sensing advances provide the opportunity for real-time control of the qubit classical environment via a novel combination of qubit sensing, statistics, machine learning, and control approaches. In the new paradigm, qubit sensor-based characterization and verification of classical control fields conducted by a distinct set of "spectator" qubits located in the vicinity of the data qubits are visualized.

The MURI team is exploring this new paradigm by investigating the potential role of spectator qubits to quantify noise in quantum systems in real time and developing control strategies for high-performance operations that can be updated based on this information. The team will aim to characterize the noise using three methods: classical detectors, sensing with the data qubit, and real-time measurement of an integrated spectator qubit.

Science of Embodied Innovation, Learning and Control

This MURI began in FY18 and was awarded to a team led by Professor Daniel Koditschek, University of Pennsylvania. The goal of this MURI is to explore the emergence of embodied learning and control within natural and synthetic systems operating in uncertain and changing environments to develop a methodology that predicts statistical synchronization patterns among intrinsic nonlinear dynamics, sensing, and actuation to enable real-time model learning and adaptation. In the long term, discoveries from this MURI may lead to new paradigms to design and develop agile and dexterous autonomous systems capable of operating in any terrain and under battlefield conditions.

Progress in agile robotics has been limited by control methods reliant on optimization about linearized passive dynamics and nearly ideal sensing. A robot's mobility depends on its capacity to move energy from a store to its mass center along the right degrees of freedom at the right time by actuating appendages toward the periphery where it meets the environment. Because there is a premium on getting this work done quickly, power (the rate at which actuators can move Joules) is a first scarce resource. The information required to direct these outward flows appropriately must also be generated from some prior memory combined with feedback decisions made using real time streams. Moreover, since the purposes of mobility are inevitably linked to the robot's knowledge about the environment as well as the task, its ability to bring information from the periphery inward to the core at adequate rates inevitably presents a challenge simultaneous with and dual to its management of outward power flows.

A key focus of this research is to uncover the design of morphology, mainly the nature of limbs and body and their endowment with actuation and perceptual resources, to promote effective interaction between energy and information streams over contrasting scales of length and time. The project also aims to discover how to evolve, use, and revise this endowment to achieve goal-directed mobility; creating new solutions to sensorimotor limitations and challenges represents the second focus.

ARL Competencies:

Humans in Complex Systems

Mechanical Sciences

MURI Author(s) and Manager(s):

Dr. Samuel Stanton, Mechanical Sciences Branch

Stimuli-Responsive Control of Protein-Based Molecular Structure

This MURI began in FY18 and was awarded to a team led by Professor Milan Mrksich, Northwestern University. The goal of this MURI is to enable dynamic control over the motion of protein domains via incorporation of stimuli-responsive dynamic bonding chemistries (excluding disulfide/thiol linkages) to control protein function. In the long term, discoveries from this MURI may lead to engineered enzymes that provide a readily accessible supply of molecules that are currently difficult or impossible to produce or protein biomaterials with tunable mechanical properties for broad applications from antibiotics to optical storage materials.

In biological systems, function is determined by structure. This structure–function relationship is particularly striking for proteins, where function is not solely determined by a static structure, but is also dependent on dynamic motions of subdomains within the folded protein. The most commonly observed domain motions are hinge and shear motions that occur in response to ligand binding, such as the hinge closure of hexokinase upon binding of glucose. To realize the full promise of engineered biological systems, mechanisms to exert dynamic control over protein structure are critical to enable regulation of protein activity.

Chemists have recently demonstrated incorporation of non-natural chemical functional groups into proteins that support synthetic bonding chemistries, including novel protecting groups that provide control over the accessibility of bonding moieties using applied external stimuli. Moreover, a variety of dynamic chemical switches have been developed for synthetic polymer systems in recent years, expanding the range of dynamic bonding chemistries that could be used for protein engineering. In recent years, a variety of dynamic bonding schemes have been introduced into synthetic polymer systems that enable triggered structural changes in response to applied stimuli, such as light, changes in pH, mechanical stress, and redox conditions. In these structurally dynamic polymers, macroscopic changes originate from a change in the polymer's molecular architecture through the controlled formation/breakage of bonds, providing a linkage between molecular structure and macroscopic properties that is not typically inherent in synthetic polymer systems. These dynamic chemical switches provide an opportunity to bring structural, and thus functional, control to protein biopolymers.

The MURI team is employing these biological and chemical principles to design reversible covalent chemistries that can be used to regulate the conformations of protein-based structures, and combine experimental and computational approaches to design and demonstrate large-scale conformational changes in protein-based structures in response to an applied stimulus.

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Stephanie McElhinny, Life Sciences Branch

Dr. Dawanne Poree, Chemical Sciences Branch

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Lisa Troyer, Life Sciences Branch

Dr. Derya Cansever, Network Sciences Branch

Toward a Multiscale Theory on Coupled Human Mobility and Environmental Change

This MURI began in FY18 and was awarded to a team led by Professor Rachata Muneepeerakul, University of Florida. The goal of this MURI is to create a theory integrating environmental change, human social system dynamics, and the corresponding interdependencies to create and validate predictive models that capture these dynamics to anticipate the trajectory of environmental change and human effects on these changes. In the long term, discoveries from this MURI may lead to new tools to advance situational awareness and facilitate operational decision-making, including the identification of emerging regions of potential conflict and risk.

Large-scale environmental changes such as floods, earthquakes, and droughts can drive social mobility, which often precipitate new population migration patterns that, in turn, affect health, crime, and sociopolitical instability as humans relocate to access critical resources. However, the ability to model, theorize, and predict the interdependencies among environmental change and human social system dynamics remains a scientific challenge. Successful models of social–natural interdependence must account for the unique temporal/spatial scales of those systems, the factors determining action, and the natural and social constraints placed on those actions. These requirements pose substantial analytic challenges that no single discipline has been able to overcome.

This project is modeling population dynamics as movements of people over multilayer networks, each with interdependencies between natural environments and social institutions (e.g., governance structures, religious belief systems, kin networks). There will be four case studies that develop the modeling through natural disasters (e.g., hurricane), degrading economic systems (e.g., inflation), and two cases that integrate natural disasters and natural crises to capture secondary pushes that accelerate migration). Consequently, the project captures a range of effects across systems, including the ability to contrast sudden shocks and gradual degradations. An important feature of the modeling and testing approach is the use of Bayesian frameworks to assess the relative contributions of global sensitivity measures and expert opinion inputs on prediction of migration pathways.

ACTIVE MURIS THAT BEGAN IN FY17

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Drs. Paul Baker and Marc Ulrich, Physics Branch

Dr. Chakrapani Varanasi, Materials Science Branch

Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene

This MURI began in FY17 and was awarded to a team led by Professor Andrea Young, University of California, Santa Barbara. The goal of this MURI is to unambiguously realize new systems exhibiting the physics of anyons and verify their topological protection against decoherence.

The unparalleled potential capabilities of quantum sensors and quantum computers hinge upon finding systems that can be well controlled and robust against decoherence. Anyons are quasiparticles with fractional quantum statistics that can exist in low-dimensional systems and whose topological properties allow one to create quantum states that are protected from many sources of decoherence. The experimental evidence of the fractional quantum Hall effect (FQHE) was a landmark demonstration of topological order and fractional (anyonic) statistics in a 2D electronic system. However, the fragility of the FQHE states, in which interesting anyons can exist, have prevented this approach from advancing despite decades of improvements in material quality. On the other hand, the recent experimental realization of Majorana modes by several groups provides an important scientific opportunity to explore these intriguing quasiparticles and provides a possible pathway to realize more general anyonic systems. Advances in 2D materials, including topological surface states, new measurement capabilities, and recent theoretical progress in analyzing strongly correlated systems are rapidly advancing toward additional breakthroughs. This MURI effort will include studies of intrinsic anyons alongside extrinsic, synthetic approaches. The realization of these new robust states can pave the way for advances in universal decoherence free quantum sensors and computation as well as provide materials with currently unachievable properties that can be explored scientifically.

Adaptive Self-Assembled Systems

This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs, University of Pittsburgh. The goal of this effort is to develop experimental and theoretical approaches to integrate microscopic forms of self-organization with a scalable means of additive 3D fabrication.

Recent research related to the bottoms-up assembly of material has demonstrated the feasibility of using tailored short-range interactions to drive the assembly of functional clusters and macromolecular assemblies that are capable of performing basic functions such as catalysis, energy harvesting, color change, and actuation. However, it is not currently possible to go beyond basic functionality and establish hierarchically ordered systems that display complex functional integration and dynamic system response. In particular, multifunctional structures with specifically targeted properties and robust feedback and control mechanisms that can embody aspects of emergent behavior and robust reconfiguration remain well beyond reach. This effort aims to establish the knowledge and expertise base needed to enable the design and directed assembly of nano-building blocks into complex, hierarchical 3D architectures capable of long-range control over multifunctional behavior and smart/dynamic responses using an additive 3D material assembly approach. The research is organized around three major thrusts: (1) assembly of microscale musculoskeletal frameworks, (2) transduction of energy to enable functionality, and (3) additive manufacturing of large-scale dynamic material systems. If successful, the research will enable the development of artificial "smart" materials and structures that exhibit tightly coupled capabilities for sensing environmental cues and then transducing energy to perform useful, situation-specific dynamic responses.

ARL Competencies:

Sciences of Extreme Materials

Electromagnetic Spectrum Sciences

Mechanical Sciences

MURI Author(s) and Manager(s):

Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Branch

Dr. Dawanne Poree, Chemical Sciences Branch

Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems

This MURI began in FY17 and was awarded to a team led by Professor Igor Mezic, University of California, Santa Barbara. The objective of this MURI is to develop a spectral decomposition theory that encompasses elements of ergodic theory, geometric theory of dynamical systems, and functional analysis via the spectral theory of linear infinite dimensional operators, control theory, machine learning for inference, prediction, and uncertainty analysis.

The MURI team approach will be to study systems in which there exists a model (e.g., the Navier–Stokes equation for fluid flow) as well as systems with no model (e.g., data streaming either from physical sensors or unstructured data). In both cases, the team will develop efficient methods to extract the correct descriptive variables via spectral properties of associated operators. The main theory topics to be pursued will expand the current reach of spectral expansion analysis: (1) stability theory for general attractors, treatment of continuous spectrum; (2) uncertainty analysis and spectral expansion theory of the Perron–Frobenius operator for observable evolution; (3) extensions to inference, prediction, and control; (4) spectral expansions for finite-time analysis; and (5) non-smooth systems. The main numerical analysis topics to be pursued will expand the current reach of spectral expansion analysis: (1) proofs of convergence of finite-dimensional approximations to spectral objects of the infinite-dimensional Koopman and Perron–Frobenius operators; (2) algorithms for finite-time analysis in nonautonomous and control systems; (3) algorithms for extraction of finite-dimensional models from data for inference, prediction and control; (4) rigorous use of machine learning algorithms in spectral expansion theory; and (5) use of spectral expansion theory for development of next-generation, real-time computational tools for complex physics with applications to vortex dynamics. Finally, the team will investigate experimental and data analysis topics to expand the current reach of spectral expansion analysis: (1) network monitoring problems arising in cybersecurity, 2) experiments in locomotion for a class of hybrid oscillators, (3) experiments on finite-time vortex stability, and (4) experiments on one of the most vexing continuous spectrum problems—turbulence in fluid–structure interactions leading to large deformations. All of these areas span DoD interests such as helicopter dynamics, robotics, and cybersecurity. These developments in this MURI will lead to a massive changes in design, data inference, and control of systems possessing a very broad set of nonlinear features.

ARL Competencies:

Mechanical Sciences

MURI Author(s) and Manager(s):

Drs. Samuel Stanton and Matthew Munson, Mechanical Sciences Branch

Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress

This MURI began in FY17 and was awarded to a team led by Professor Elaine Hsiao, University of California, Los Angeles. The objective of this MURI effort is to investigate how the community of microorganisms naturally residing in the human gut (i.e., the gut microbiome) alters cognitive performance in response to nutritional and physical stress.

Recent studies from several laboratories reveal that the responses of the human microbiome, and specifically the gut microbiome, respond to environmental factors (e.g., diet and stress) in a way that modulates host brain activity and behavior. The objective of this MURI is to uncover gut

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

MURI Author(s) and Manager(s):

Drs. Frederick Gregory and Robert Kokoska, Life Sciences Branch

microbiome influence on host neurobiology; develop a layered cellular and systems-level model and theory of cognitive and behavioral control by commensal gut microorganisms; and extract integrated neural, endocrine, immune and gut microbial interaction principles governing nutrition and physical stress response.

This MURI, if successful, will provide sophisticated predictive tools available to the academic community and DoD upon which more comprehensive biological studies could be performed to more completely understand causative effects throughout this complex networked system. These models have the potential to far exceed current state of the art by offering a currently unavailable analytical framework for future discoveries. The long-term potential applications could be the rational design of probiotic regimens to ameliorate symptoms of anxiety-like disorders including PTSD and methods to manipulate the gut microbiome to affect human performance without the need for genetically engineering the human host. Outcomes of this MURI would also direct whole-force recommendations to the Army Surgeon General's Performance Triad and Brain Health Campaigns.

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Cliff Wang, Network Sciences Branch

Dr. Lisa Troyer, Life Sciences Branch

Realizing Cyber Inception: Toward a Science of Personalized Deception for Cyber Defense

This MURI began in FY17 and was awarded to a team led by Professor Milind Tambe, University of Southern California. The goal of this MURI research is to gain scientific understandings to significantly advance the state of art in learning and modeling of adversarial mental states and decision processes to create metrics quantifying information effectiveness in driving cognitive state change under the deception context, and build an integrated framework of deception composition and projection methods to successfully manipulate adversaries' mental state and decision-making process to our advantages.

The research focuses on an innovative and comprehensive study of adaptive cognitive modeling, cyber deceptive game theory, and deception and monitoring systems. The effort consists of three major thrusts. (1) Deception and monitoring systems: ultimately deceptive strategies developed by higher-level reasoning about the attacker must be realized in a system in such a way that the deceptions are convincing and their effects on the attacker can be effectively monitored. (2) Cyber-deceptive game theory: game theory provides a mathematical framework for modeling the interactions between defenders and attackers in cybersecurity, which is an important foundation for developing a science of security. Developing game-theoretic models and algorithms for cybersecurity will allow richer modeling of adversarial interactions, a deeper understanding of deception and information manipulation tactics, and more effective response strategies. (3) Cognitive modeling: cognitive models provide a computational representation of human cognitive processes, their detailed mechanisms and limitations, and the knowledge upon which they operate. By taking advantage of human-bounded rational decision behavior, where humans make decisions according to the constraints on the environment of their own cognitive limitation, the team will build a personalized model of adversary behavior.

ARL Competencies:

Sciences of Extreme Materials

Photonics, Electronics, and Quantum Sciences

Military Information Sciences

MURI Author(s) and Manager(s):

Dr. Michael Gerhold, Electronics Branch

Dr. Marc Ulrich, Physics Branch

Room-Temperature Exciton-Polaritonics

The MURI began in FY17 and was awarded to a team led by Professor Hui Deng, University of Michigan. The goal of this effort is to explore the use of 2D materials for exciton-polariton systems. Such materials have large exciton binding energies that indicate room temperature operation may be possible.

Research on 2D materials known as transition metal dichalcogenides (TMDs) has progressed to a degree where the development of Bose-Einstein condensates of exciton-polaritons, which form a coherent light-matter interactive state, is feasible. Such condensates have been shown to emit coherent radiation, equivalent to a laser, at much lower carrier densities than typical photon lasers. Integrated photonics platforms that utilize coherent light could benefit from such room-temperature light sources. The transport of the condensates themselves could also effectively lead to a form of superconductivity for the charged carriers due to the dissipationless propagation of the photonic part of the exciton-polariton. Therefore, exciton-polariton platforms could carry out a number of functions found on photonic circuit platforms but operate at low energies. Important applications for the polariton regimes include short distance optical interconnects, neuromorphic information processing and computing, and ultra-low energy sensing.

One of the key objectives of Professor Deng's effort is to explore 2D material science improvements. Specifically, increasing the grain-size and production of transferrable 2D nanosheets for integration with microcavities. Another objective of this effort focuses on understanding the stacking behavior of the 2D materials to create nanostructures and interlayer excitons for ultra-low energy effects related to switching and polariton control. The research team will also focus on understanding how organic materials determines hybrid TMD-organic polariton effects. The team will pursue these goals by combining state-of-the-art fabrication capabilities with strong experimental and theoretical expertise on polariton physics, 2D materials, photonic devices, and many-body physics in photonic and electronic systems.

Semantic Information Pursuit for Multimodal Data Analysis

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Hamid Krim, Computing Sciences Branch

This MURI began in FY17 and was awarded to a team led by Professor Rene Vidal, Johns Hopkins University. The goal of this research is to establish the theoretical foundation for context and principles of information physics for data analysis that provide an analytical framework and computation algorithms for the characterization, analysis, and understanding of information content in multimodal data.

The proposed information-theoretic framework for characterizing information content in multimodal data combines principles from information physics with probabilistic models that capture rich semantic and contextual relationships between data modalities and tasks. These information measures will be used to develop novel statistical methods for deriving minimal sufficient representations of multimodal data that are invariant to some nuisance factors as well as novel domain adaptation techniques that mitigate the impact of data transformations on information content by finding optimal data transformations. The computation of such optimal representations and transformations for classification and perception tasks will require solving nonconvex optimization problems, for which novel optimization algorithms with provable guarantees of convergence and global optimality will be developed. The uncertainty of such information representations derived from multimodal data will be characterized via novel statistical sampling methods that are broadly applicable to various representation learning problems. The information representations obtained from multiple modalities will be integrated by using a novel information theoretic approach to multimodal data analysis called information pursuit, which uses a Bayesian model of the scene to determine what evidence to acquire from multiple data modalities, scales, and locations, and coherently integrate this evidence. The proposed methods will be evaluated in various complex multimodal datasets, including text, images, video, cellphone data, and body-worn cameras.

ACTIVE MURIS THAT BEGAN IN FY16

Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Hamid Krim, Computing Sciences Branch

Dr. Frederick Gregory, Life Sciences Branch

This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi, University of Southern California. The goal of this research is to create new methodologies for modeling multimodal neural activity underlying multisensory processing and decision-making, and use those methodologies to design closed-loop adaptive algorithms for optimized exploitation of multisensory data for brain–computer communication.

This research effort will contribute to the development of a new closed-loop brain–computer interface (BCI) framework for enhancing decision accuracy. The framework will collect multimodal neural, physiological, and behavioral data; decode mental states such as attention orientation and situational awareness; and use the decoded states as feedback to adaptively change the multisensory cues provided to the subject, thus closing the loop. To realize such a framework, the effort will make fundamental advances on four fronts, constituting four research thrusts: (1) modeling multisensory integration, attention, and decision-making, and the associated neural mechanisms; (2) machine learning algorithms for high-dimensional multimodal data fusion; (3) adaptive tracking of the neural and behavioral models during online operation of the BCI; and (4) adaptive BCI control of multisensory cues for optimized performance. Complementary experiments with rodents, monkeys, and humans will be conducted to collect multimodal data to study and model multisensory integration, attention, and decision-making, and prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and machine learning to develop (1) novel Bayesian and control-theoretic models of the brain mechanisms, (2) new stochastic models of multimodal data and adaptive inference algorithms for this data, and (3) novel adaptive stochastic controllers of multisensory cues based on the feedback of users' cognitive state.

Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Frederick Gregory, Life Sciences Branch

Dr. Virginia Pasour, Mathematical Sciences Branch

This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton, University of California, Santa Barbara. The goal of this MURI is to uncover the temporal dynamics of neural substrates and cognitive processes engaged during skill learning and generate a definition of expertise based on the underlying neurocognitive computational advantages generated through learning.

Neuroscience, social psychology, and education are providing insights into neural and cognitive processes involved during skill learning, which show structural and functional differences in multiple brain regions when compared between "experts" and "novices." Typically, these comparisons involved a novice time point and an expert time point because of the difficulty measuring intracranial brain activity over the course of skill learning. Novel materials now enable long-term implantation of high-density neural recording devices in humans and animal models. Emerging engineering breakthroughs enable spike and local field potential recording from multiple neuroanatomical sites in the brain simultaneously. However, a major analytical barrier prevents easily linking this high-density data with data acquired through existing noninvasive electrophysiology techniques and other tools for determining structure–function relationships, like magnetic resonance imaging.

The objective of this research is to develop tools and techniques that can both predict and explain from a neurobiological perspective why there are differences among individuals in their ability to develop expertise. The future force demands expert Soldier performance across many tasks. In the long term, this basic research effort will provide a critical foundation for developing training methods based on computational and network neuroscience that are grounded in neurophysiology and neuroanatomy.

Discovering Hidden Phases with Electromagnetic Excitation

ARL Competencies:

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. Marc Ulrich, Physics Branch

Dr. Chakrapani Varanasi, Materials Science Branch

This MURI began in FY16 and was awarded to a team led by Professor David Hsieh, California Institute of Technology. The goal of this project is to create new electronic states of matter that are unobtainable through conventional solid-state synthesis, which, in the long term, may lead to enhancements of electronic, optical, magnetic, and thermal material properties that would lay a foundation for future technology in many areas.

Nascent research has demonstrated unique phases that are not adiabatically accessible from the known phase diagram. Recent discoveries have involved photo-excitation of a material with an ultra-short pulse that non-adiabatically induces a phase distinct from that existing elsewhere on the ground-state phase diagram. Examples include a nonequilibrium superconducting state in a BCS superconductor, a ferromagnetic state in an antiferromagnetic oxide, and a unique metallic state in a thin film of a dichalcogenide. The team is attempting to employ excitations across the entire electromagnetic (EM) spectrum, including with extremely high pulsed fields, to design, realize, and manipulate new phases and responses in strongly correlated materials. Specifically, the team will focus on realizing new correlated states via the following approaches: (1) EM-stimulated, bond-selective tuning of charge-hopping parameters; (2) direct EM modification of magnetic exchange, order, and frustration; (3) continuous EM control of dimensionality and hybridization; and (4) EM excitation across kinetic barriers to realize metastable states that are thermodynamically inaccessible. Using these nonequilibrium methods, they will aim at realizing some of the most sought-after phenomena in condensed-matter physics including collective charge/current ordered phases, bandwidth-controlled metal to Mott insulator transitions, quantum disordered magnets such as valence bond solids and highly entangled quantum spin liquid states, and low-dimensional and quantum critical electron liquids with no quasiparticle description.

Modular Quantum Systems

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

This MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe, University of Maryland, College Park. The goal of this research is to discover and explore modularity concepts for extensibility of small high-performance, multi-qubit systems to larger systems with reduction of operational complexity.

A paramount challenge in exploring physical systems (qubits) suitable for quantum information processing has been the contradictory requirement for precise manipulation of a quantum state on demand while maintaining strict isolation from the environment. Significant progress has been made in addressing this challenge. Coherence in several physical qubit types has improved by orders of magnitude. High-fidelity fundamental quantum logic operations have been demonstrated. This progress has extended to multi-qubit systems involving a few (order ten) qubits. Progress continues to be made in improving coherence and fidelity. In parallel, advances have been made in connecting physically separated qubits. Key to these rapid advances has been a multidisciplinary approach involving physics, materials science, control engineering, computer science, and mathematics, among other fields. A scientific challenge to further progress in the field has been the difficulty to add qubits and increase system size, while maintaining coherence and high-fidelity operations. System size needs to be increased before useful functionality can be explored and realized. Adding qubits increases the complexity of interactions between the qubits and makes layout, fabrication, and quantum control for high-fidelity operations extremely challenging. Additional unwanted interactions introduce new qubit degrees of freedom to entangle with the environment and degrade coherence and fidelity. Modularity is a general scientific approach to address such complexity, in which the system is decomposed into repeatable blocks with well-defined and controlled interfaces and interactions between the blocks, and has been applied successfully to classical systems. Here, a module can be envisaged as a functional group of qubits and an interface. Exploring modularity for complex quantum systems is nascent but provides a potential extensible approach in which small numbers of high-performance qubits can be extended to groups of high-performance qubits and interfaces capable of precise manipulation within the group, between groups when required, and isolation from the environment and other groups.

Any quantum information processing system must balance the need for coherent control of the many interacting qubits necessary for a large-scale quantum system with decoherence rates that generally grow with system size. The objective of this research is to investigate a modular approach to constructing multi-qubit systems suitable for quantum information processing to determine whether a modular system can achieve this balance, and study the associated costs and benefits of taking the approach. In the long term, this research may overcome barriers and lead to new capabilities in the logistics, optimization, and the quantum simulation of materials.

MURI Author(s) and Manager(s):

Dr. T. R. Govindan, Physics Branch

Dr. T. Curcic, Air Force Office of Scientific Research

Multimodal Energy Flow at Atomically Engineered Interfaces

ARL Competencies:

Energy Sciences

This MURI began in FY16 and was awarded to a team led by Professor Donald Brenner, North Carolina State University (initially led by Professor Jon Paul Maria). The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale nonequilibrium phenomena at and across materials interfaces, especially the flow, redistribution, and partition of energy near the interface, by devising and applying novel experimental, theoretical, and simulation approaches.

The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-nonequilibrium excitations within nanoscale geometries, observe in situ picosecond to microsecond property responses using newly developed methods, inform new theoretical models, and enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and predict their performance.

MURI Author(s) and Manager(s):

Dr. Ralph Anthenien, Mechanical Sciences Branch

Dr. Robert Mantz, Chemical Sciences Branch

Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery

ARL Competencies:

Biological and Biotechnology Sciences

This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett, Northwestern University. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using nontraditional chain growth polycondensation chemistries (beyond amide and ester linkages).

Employing only 4 nucleotides and 20 amino acids, a plethora of biopolymers (e.g., proteins, DNA) with a precisely defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building

MURI Author(s) and Manager(s):

Dr. Dawanne Poree, Chemical Sciences Branch

Dr. Stephanie McElhinny, Life Sciences Branch

ARO IN THE NEWS

Army project may lead to new class of high-performance materials

By U.S. Army CCDC Army Research Laboratory Public Affairs
November 18, 2019

Synthetic biologists working on a U.S. Army project have developed a process that could lead to a new class of synthetic polymers that may create new high-performance materials and therapeutics for Soldiers.

Nature Communications published research conducted by Army-funded researchers at Northwestern University, who developed a set of design rules to guide how ribosomes, a cell structure that makes protein, can incorporate new kinds of monomers, which can be bonded with identical molecules to form polymers.

> **"These findings are an exciting step forward to achieving sequence-defined synthetic polymers, which has been a grand challenge in the field of polymer chemistry," said Dr. Dawanne Poree, program manager, polymer chemistry at the Army Research Office. "The ability to harness and adapt cellular machinery to produce non-biological polymers would, in essence, bring synthetic materials into the realm of biological functions. This could render advanced, high-performance materials such as nanoelectronics, self-healing materials, and other materials of interest for the Army."**

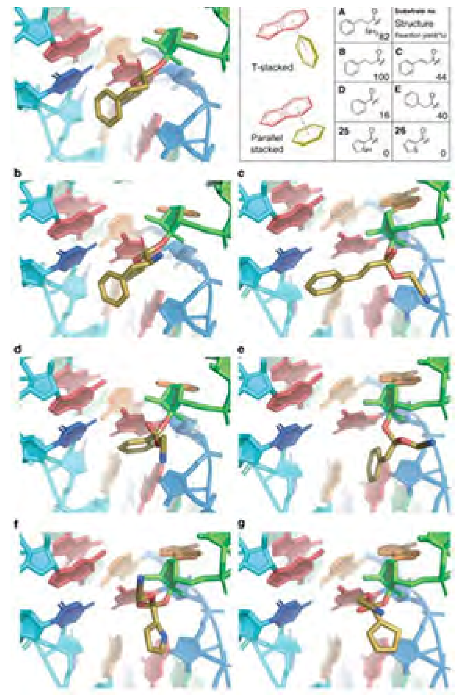
Biological polymers such as DNA, have precise building block sequences that provide for a variety of advanced functions such as information storage and self-replication. This project looked at how to re-engineer biological machinery to allow it to work with non-biological building blocks that would offer a route to creating synthetic polymers with the precision of biology.

> **"These new synthetic polymers may enable the development of advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells and nanofabrication, which are all key to the protection and performance of Soldiers," Poree said.**

"We set out to expand the range of ribosomal monomers for protein synthesis to enable new directions in biomanufacturing," said Michael Jewett, the Charles Deering McCormick Professor of Teaching Excellence, professor of chemical and biological engineering, and director of the Center for Synthetic Biology at Northwestern's McCormick School of Engineering. "What's so exciting is that we learned the ribosome can accommodate more kinds of monomers than we expected, which sets the stage for using the ribosome as a general machine to create classes of materials and medicines that haven't been synthesized before."

Recombinant protein production by the ribosome has transformed the lives of millions of people through the synthesis of biopharmaceuticals, like insulin, and industrial enzymes that are used in laundry detergents. In nature, however, the ribosome only incorporates natural amino acid monomers into protein polymers.

To expand the repertoire of monomers used by the ribosome, Jewett's team set out to identify design rules for linking monomers to Transfer ribonucleic acid, known as tRNAs. That is because getting the ribosome to



use a new monomer is not as simple as introducing a new monomer to the ribosome. The monomers must be attached to tRNAs, which are the molecules that carry them into the ribosome. Many current processes for attaching monomers to tRNAs are difficult and time-consuming, but a relatively new process called flexizyme enables easier and more flexible attachment of monomers.

To develop the design rules for using flexizyme, the researchers created 37 monomers that were new to the ribosome from a diverse repertoire of scaffolds. Then, they showed that the monomers that could be attached to tRNAs could be used to make tens of new peptide hybrids. Finally, they validated their design rules by predictably guiding the search for even more new monomers.

> **"With the new design rules, we show that we can avoid the trial-and-error approaches that have been historically associated with developing new monomers for use by the ribosome," Jewett said.**

These new design rules should accelerate the pace in which researchers can incorporate new monomers, which ultimately will lead to new bioproducts synthesized by the ribosome. For example, materials made of protease-resistant monomers could lead to antimicrobial drugs that combat rising antibiotic resistance.

The research is part of the Department of Defense's Multidisciplinary University Research Initiatives program, supported by ARO, in which Jewett is working with researchers from three other universities to reengineer the ribosome as a biological catalyst to make novel chemical polymers. ARO is an element of the U.S. Army Combat Capabilities Development Command's Army Research Laboratory.

"It's amazing that the ribosome can accommodate the breadth of monomers we showed," Jewett said. "That's really encouraging for future efforts to repurpose ribosomes."

Researchers at the University of Texas at Austin are working on a similar technology to develop adhesion and adaptive and responsive materials as part of a cooperative agreement with ARL and Army Futures Command.

blocks, has many scientific and technological implications, as it would enable precise control over structure–property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of Soldiers.

For more information on this effort, check out the ARO in the News feature on the preceding page!

Spin Textures and Dynamics Induced by Spin-Orbit Coupling

ARL Competencies:

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. Joe Qiu, Electronics Branch

Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Branch

Dr. Marc Ulrich, Physics Branch

This MURI began in FY16 and is led by Professor Kang Wang, University of California, Los Angles. The team consists of researchers from the University of California, Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas at Austin. The objective of this project is to strive for understanding of interfacial spin-orbit coupling (SOC) and exchange coupling in novel heterostructures and superlattices of topological insulators (TIs), 2D transition metal dichalcogenides (TMDs), and ferromagnetic (FM)/ferri-magnetic/antiferromagnetic (AFM) materials. High-quality heterostructures and superlattices containing TI/TMDs, TI/FM, and TI/AFM with the atomically sharp interface are to be synthesized and characterized, and these will constitute an ideal laboratory for enabling understanding of the interfacial SOC effects and relevant spin textures and dynamics.

This project will exploit the symmetry breaking and SOC-induced collective properties (i.e., magnetization, spin wave, and spin-orbit torque) in these heterostructures and superlattices to realize new types of topological matters such as magnetic Skyrmions, topological valley insulators, and topological spin wave (magnonic) crystals. It will also help facilitate the development of new emerging fields including spin-orbitronics, spin-valley-tronics, and axion electrodynamics. In addition, direct electrical-field manipulation of spin or magnetization textures in these proposed systems through spin-orbit torque and magnetoelectric effects will be investigated for energy efficiency. The anticipated results of this project will broaden understandings of the fundamental science enabled by SOC and establish suitable material frameworks for new spin-orbitronic devices in which multi-functional applications of spintronics for ultra-low-power electronics at terahertz can be realized. This research will set a milestone in the spin-based applications by creating the knowledge base to enable novel, fast, and energy-efficient technologies for communications and information processing.

Socio-Cultural Attitudinal Networks

ARL Competencies:

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Purush Iyer, Computing Sciences Branch

Dr. Lisa Troyer, Life Sciences Branch

This MURI began in FY16 and was awarded to a team led by Professor Larry Davis, University of Maryland (initially led by Professor V. S. Subrahmanian). The goal of this MURI is twofold: (1) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive and (2) develop multimedia analytics tools that formalize those social science theories as algorithms, which can aid an observer who is not steeped in the local culture.

While driven by practical problems, the objectives of the proposed work is not only to drive the development of new social science theories, but also drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.

ACTIVE MURIS THAT BEGAN IN FY15

Advanced 2D Organic Networks

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Chakrapani Varanasi,
Materials Science Branch

Dr. Dawanne Poree,
Chemical Sciences Branch

This MURI began in FY15 and was granted to a team led by Professor William Dichtel, Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically, the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

Emulating the Principles of Impulsive Biological Force Generation

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Samuel Stanton,
Mechanical Sciences Branch

Dr. Robert Kokoska,
Life Sciences Branch

This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek, Duke University. The objective of this MURI is to establish a unified theory for understanding biological and engineered impulsive systems.

The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force–velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales, and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification)—a defining feature of impulsive systems—through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation, and reset mechanisms for repeated use and mitigation of failure due to environmental forces.

This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials.

Engineering Exotic States of Light with Superconducting Circuits

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. T. R. Govindan, Physics Branch

Dr. Joe Qiu, Electronics Branch

This MURI began in FY15 and was awarded to a team led by Professor Andrew Houck, Princeton University. The goal of this MURI is to initiate significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. If successful, this research may lead to new tools for metrology, could provide key insight into nonequilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon–photon interactions, high photon loss introduces decoherence, and low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single-shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of hundreds of photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology, could provide key insight into nonequilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Joseph Myers, Mathematical Sciences Branch

This MURI began in FY15 and is awarded to a team led by Professor George Karniadakis, Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (1) mathematical analysis of FPDEs; (2) numerical approximation of FPDEs; (3) development of fast solvers; (4) fractional order estimation and validation, from data; and (5) prototype application problems.

Imaging and Control of Biological Transduction using Nitrogen-Vacancy Diamond

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Frederick Gregory, Life Sciences Branch

Dr. Paul Baker, Physics Branch

This MURI began in FY15 and was awarded to a team led by Professor Ronald Walsworth, Harvard University. The goal of this MURI is to further develop N-V nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes.

The N-V center lattice defect in diamond nanoparticles (N-V-diamond) can retain activity in biological environments. Current applications of N-V-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging, and atomic-scale magnetic resonance imaging. These state-of-the-art applications involve N-V-diamonds implanted in substrates; however, recent breakthroughs have allowed isolated nanodiamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for N-V-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from N-V-diamond are sensitive to external perturbation by strain, temperature, electric fields, and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent demonstrations of N-V-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning N-V-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project four closely coupled aims to (1) optimize N-V-nanodiamond synthesis, (2) realize stable, biocompatible nanodiamond surface functionalizations, (3) advance N-V sensitivity to chemical and biological systems, and (4) enable N-V-based manipulation of biological transduction. Systematically studying the integration of N-V nanodiamonds with reconstituted or native ion channels will lead to greater understanding and, more importantly, create a new paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. This endeavor may lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, this research may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular level, novel human–machine interfaces, and antidotes to neurotoxins and pathogens.

Multiscale Responses in Organized Assemblies

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Dawanne Poree,
Chemical Sciences Branch

Dr. Evan Runnerstrom (initially managed by Dr. John Prater),
Materials Science Branch

This MURI began in FY15 and was awarded to a team led by Professor Sankaran Thayumanavan, University of Massachusetts Amherst. The goal of this MURI is understanding how a molecular-level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multiscale events to realize signal amplification.

Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal–propagate–response pathway are inadequately understood to rationally design autonomous, "living" systems. The daunting challenge toward synthetic "living" systems is predictably propagating a molecular-level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material's fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multiscale levels—from molecular to nano to macroscopic length scales, and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multiscale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid-crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with nonequilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well formulated, and focused on a complete understanding of the basic research principles controlling each approach. A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes. A key part of this effort is the ability to monitor dynamic changes during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy. If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

Network Science of Teams

This MURI began in FY15 and was awarded to Professor Ambuj Singh, University of California, Santa Barbara, with participation from researchers at the University of Southern California, University of Illinois Urbana-Champaign, Northwestern University, and MIT. These seven faculty provide an excellent balance of multidisciplinary scholars from sociology, cognitive and social psychology, health and behavioral sciences, computer science, statistics, controls and dynamical systems, and network science. This MURI will advance the development of the network science of teams by creating quantitative, network-based models of adaptive team behavior.

This research will produce methods to optimize team performance under different contexts and resource constraints. The three thrusts of this research effort include (1) teams as networks of interacting entities, (2) analysis and models of dynamic team behavior over task sequences, and (3) the network science of teams-of-teams or multi-team systems. The overarching objectives of this research are to build quantifiable informative models of team behavior as dynamical systems interacting over multiple networks, develop rigorous models that relate interaction patterns and network evolution to task performance, break new ground in the learning of optimal design of teams for complex tasks, and advance social science theories of team performance. This MURI will have a significant impact for the Army and DoD with respect to how it conducts its work in teams in that results from this research may help the Army and joint forces assemble more effective teams and teams of teams, and provide guidance on task sequencing to support their highest goals.

ARL Competencies:

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Edward Palazzolo, Network Sciences Branch

Noncommutativity in Interdependent Multimodal Data Analysis

This MURI began in FY15 and was awarded to a team led by Professor Rayadurgam Srikant, University of Illinois Urbana-Champaign (initially led by Professor Negar Kiyavash). The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing.

Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including (1) human action and collective behavior recognition and (2) crowdsourcing in a network of brain–machine interfaces. The framework will provide answers to questions such as the following: What are the fundamental performance limits for noncommutative information collection and processing systems? What is the effect of side information on noncommutative information structures? How can low-complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include, but are not limited to, introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision-making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain–computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

ARL Competencies:

Humans in Complex Systems

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Hamid Krim, Computing Sciences Branch

Dr. T. R. Govindan, Physics Branch

ACTIVE MURIS THAT BEGAN IN FY14

Attosecond Electron Dynamics

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

MURI Author(s) and Manager(s):

Dr. James Parker, Chemical Sciences Branch

Dr. Marc Ulrich, Physics Branch

This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone, University of California, Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules.

Attosecond dynamics is a new field of scientific investigation that allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semiconductor materials. A recent scientific breakthrough, known as double optical gating, has led to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond timescales for the real-time observation, control, and understanding of electronic motion in atoms, molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically enhanced catalysis for the direct reduction of carbon dioxide (CO_2) to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

Force-Activated Synthetic Biology

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Stephanie McElhinny, Life Sciences Branch

Dr. Daniel Cole (initially managed by Dr. David Stepp), Materials Science Branch

This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel, University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical, and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO-funded research, including a prior MURI. Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by mechanical force into the growing toolbox of synthetic biology, and establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive biomimetic material systems.

Innovation in Prokaryotic Evolution

ARL Competencies:

Biological and Biotechnology Sciences

This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch, Indiana University Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally validated, mathematically rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage; and new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

MURI Author(s) and Manager(s):

Dr. Micheline Strand, Life Sciences Branch

Dr. Joseph Myers (initially managed by Dr. John Lavery), Mathematical Sciences Branch

Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials

This MURI began in FY14 and was awarded to a team led by Professor Mitchell Luskin, University of Minnesota. This research is co-managed by the Mathematical Sciences and Materials Science Branches. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and macroscopic continuum for layered heterostructures.

Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal, and mechanical properties. The vast range of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can, in turn, inform, refine, and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly linked multiscale methods for coupling several scales based on a rigorous mathematical basis by specifically pursuing the following: (1) the rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures; (2) the coupling of the atomistic-to-continuum will be achieved by methods that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores; (3) new accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the timescales necessary for synthesis and processing by chemical vapor deposition (CVD) and molecular beam epitaxy (MBE); and (4) the simulations will be linked to macro and electromagnetic modeling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

ARL Competencies:

Sciences of Extreme Materials

Network Science and Computational Sciences

MURI Author(s) and Manager(s):

Dr. Joseph Myers, Mathematical Sciences Branch

Dr. Chakrapani Varanasi, Materials Science Branch

Multistep Catalysis

This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer, University of Utah. The goal of this MURI is to enable multistep chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products.

The Krebs cycle is an exquisite example of a regulated enzyme cascade, which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multistep reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multistep reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multistep catalysis.

ARL Competencies:

Biological and Biotechnology Sciences

Energy Sciences

MURI Author(s) and Manager(s):

Dr. Robert Mantz, Chemical Sciences Branch

Dr. Daniel Cole (initially managed by Dr. David Stepp), Materials Science Branch

In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

Ultra-Cold Molecular Ion Reactions

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Dr. Paul Baker, Physics Branch

Dr. James Parker, Chemical Sciences Branch

This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson, University of California, Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultra-cold chemical reactions.

Investments in quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments, state preparation and readout is potentially cleaner, and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit a long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

Understanding the Skin Microbiome

ARL Competencies:

Biological and Biotechnology Sciences

Humans in Complex Systems

MURI Author(s) and Manager(s):

Dr. Virginia Pasour, Mathematical Sciences Branch

Dr. Robert Kokoska (initially managed by Dr. Wallace Buchholz), Life Sciences Branch

This MURI began in FY14 and was awarded to a team led by Professor David Karig, Applied Physics Lab at Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and show how this understanding can be used to identify disease risk, predict disease outcomes, and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result, there are no effective tools to predict individuals more likely to acquire skin bacterial infections and then determine the efficacy of forensic analyses based on skin bacterial communities or design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry, and synthetic biology will be used to probe smaller-scale processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome. A series of models concentrating on four grand challenges will be built, tested, and refined: (1) predicting microbiome composition based on environmental conditions, host state, and microbe exposure patterns; (2) identifying microbiome composition through volatile sensing; (3) identifying disease risk through analysis of current state and anticipation of state changes (e.g., due to upcoming activities or events); and (4) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

ACTIVE MURIS THAT BEGAN IN FY13

Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation

ARL Competencies:

Military Information Sciences

MURI Author(s) and Manager(s):

Dr. Cliff Wang, Network Sciences Branch

This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia, George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software systems, and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called adaptive cyber defense (ACD) that will force adversaries to continually reassess, reengineer, and relaunch their cyber attacks. ACD presents adversaries with optimized dynamically changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

Artificial Cells for a Novel Synthetic Biology Chassis

ARL Competencies:

Biological and Biotechnology Sciences

MURI Author(s) and Manager(s):

Dr. Stephanie McElhinny,
Life Sciences Branch

Dr. Dawanne Poree (initially managed by Dr. Jennifer Becker), Chemical Sciences Branch

This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj, University of California, San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as a chassis for the engineered biological systems and devices. While single-celled organisms are typically used as a synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells that contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

Nanoscale Control, Computing, and Communication Far-From-Equilibrium

ARL Competencies:

Military Information Sciences

MURI Author(s) and Manager(s):

Dr. Samuel Stanton,
Mechanical Sciences Branch

This MURI began in FY13 and was awarded to a team led by Professor James Crutchfield, University of California, Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy.

Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (1) quantify the intrinsic computation in nanoscale thermodynamic systems, (2) produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (3) accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy-efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

MURI Author(s) and Manager(s):

Drs. Paul Baker and Marc Ulrich, Physics Branch

Nonequilibrium Many-Body Dynamics

This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin, University of Chicago. The goal of this MURI is to study fundamental nonequilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Nonequilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at nonequilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties. Another example is in biochemistry, in determining the role that nonequilibrium phase transitions play in driven biochemical networks—canonical phosphorylation-dephosphorylation systems with feedback that exhibit bistability. Despite the ubiquitous nature of nonequilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from nonequilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that nonequilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

ARL Competencies:

Sciences of Extreme Materials

MURI Author(s) and Manager(s):

Dr. James Parker, Chemical Sciences Branch

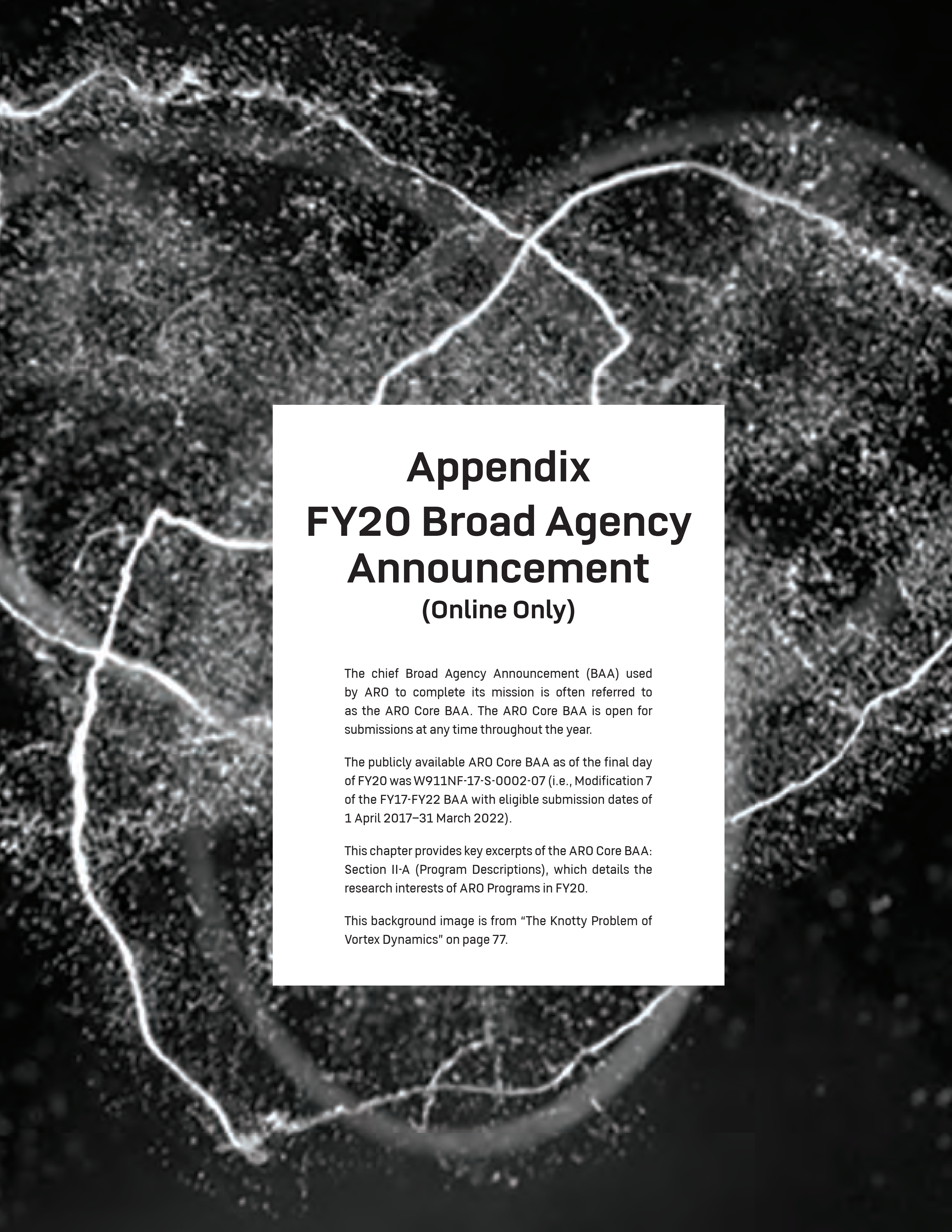
Dr. Chakrapani Varanasi, Materials Science Branch

Theory and Experiment of Co-Crystals: Principles, Synthesis, and Properties

This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger, University of Michigan. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macroscale performance of many materials, ranging from energetic materials, to pharmaceuticals, to nonlinear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on noncovalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure "parent" crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and nonlinear optical materials.



Appendix
FY20 Broad Agency Announcement
(Online Only)

The chief Broad Agency Announcement (BAA) used by ARO to complete its mission is often referred to as the ARO Core BAA. The ARO Core BAA is open for submissions at any time throughout the year.

The publicly available ARO Core BAA as of the final day of FY20 was W911NF-17-S-0002-07 (i.e., Modification 7 of the FY17-FY22 BAA with eligible submission dates of 1 April 2017–31 March 2022).

This chapter provides key excerpts of the ARO Core BAA: Section II-A (Program Descriptions), which details the research interests of ARO Programs in FY20.

This background image is from “The Knotty Problem of Vortex Dynamics” on page 77.

II. DETAILED INFORMATION ABOUT THE FUNDING OPPORTUNITY

A. Program Description

1. RESEARCH INTERESTS FOR U.S. INSTITUTIONS

ARL's ARO mission is to serve as the Army's principal extramural basic research agency funding research at universities, companies and not-for- profits in the engineering, physical, and information sciences. ARO's research portfolio is executed through ten scientific divisions, with titles reflecting fundamental scientific disciplines familiar to academic institutions. These Divisions directly support the ARL Core Technical Competencies. Additional information about the ARL S&T Core Technical Competencies can be found at the ARL website: www.arl.army.mil.

a. Physical Sciences

Research in the Physical Sciences is focused on basic research to discover, understand, and exploit physical, chemical, and biological phenomena. This research is of a fundamental nature; however, in the long term, discoveries in this area are expected to lead to revolutionary new capabilities in warfighter performance, intelligence, synthetic biology, sensing, communications, protection, power/energy storage and generation, and materials that extend the performance of Army systems well beyond current limits.

i. Chemical Sciences

The objective of the Chemical Sciences Division is to uncover and exploit the fundamental properties and processes governing molecules and their interactions in materials and chemical systems. The Division encourages proposals that promote basic research to develop methods for accurately predicting the pathways, intermediates, and energy transfer of specific reactions, to understand the fundamental processes governing electrochemical reactions and transport of species, and to discover the relationships between macromolecular microstructure, architecture, functionality, and macroscopic properties. In addition, these efforts will likely lead to new methods for synthesizing and analyzing molecules and materials that will open the door to future studies not feasible with current approaches.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in chemical sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Polymer Chemistry

The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties.

Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) *Precision Polymeric Materials* and (ii) *Complex Adaptive Polymeric Systems*. Within these thrusts, high-risk, high-payoff research is identified and supported to pursue the Program's long-term goal.

The *Precision Polymeric Materials* thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure, architecture, and functional group location. Of particular interest are research efforts that focus on novel methods for achieving sequence and tacticity control in synthetic polymers as well as enabling the synthesis of novel 2D organic polymers. Also of interest to this thrust are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures as well as influence interactions with other materials (e.g., inorganic or biological materials) to render functional hybrid assemblies.

The *Complex Adaptive Polymeric Systems* thrust focuses on developing polymers that exhibit programmed molecular responses to external stimuli. Particularly of interest are research efforts related to stimuli-responsive self-immolative polymers, polymer mechanochemistry, and stimuli-mediated polymer assembly. Additionally, research focused on exploring the assembly/incorporation of multiple responsive groups into a single polymeric material system as well as the incorporation of feedback mechanisms to engender complex responsive behavior is also of interest.

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(2) Electrochemistry

This Program supports fundamental electrochemical studies to understand and control the physics and chemistry that govern electrochemical redox reactions and transport of species, and how these are coupled with electrode, catalysis, electrolyte, and interface. Research includes ionic conduction in electrolytes, electrocatalysis, interfacial electron transfer, transport through coatings, surface films and polymer electrolytes, activation of carbon-hydrogen and carbon-carbon bonds, and spectroscopic techniques that selectively probe electrode surfaces and electrode-electrolyte interfaces. Novel electrochemical synthesis, investigations into the effect of microenvironment on chemical reactivity, quantitative models of electrochemical systems, and electrochemistry using excited electrons are also of interest.

This Program is divided into two research thrusts, although other areas of electrochemical research may be considered: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species.

The *Redox Chemistry and Electrocatalysis* thrust supports research to understand how material and morphology affect electron transfer and electrocatalysis, to tailor electrodes and electrocatalysts at a molecular level, and to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces.

The *Transport of Electroactive Species* thrust supports research to uncover the mechanisms of transport through heterogeneous, charged environments such as polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and to explore new methodologies and computational approaches to study the selective transport of species in charged environments.

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(3) Molecular Structure and Dynamics

The goal of the Molecular Structure and Dynamics program is to determine the reactive pathways and intermediates for reactions of molecules and molecular ions in gas and condensed phases at a range of temperatures and pressures, and to develop theories that are capable of accurately and efficiently describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program is divided into three research thrusts: (i) *Reaction Dynamics*, (ii) *Computational Modeling*, and (iii) *Chemistry of Novel Energetic Materials*.

Research in the *Reaction Dynamics* thrust explores energy transfer mechanisms in molecular systems. In particular, research is focused on understanding dynamic processes such as roaming radicals, chemical reactions in solid state crystals and heterogeneous mixtures, phase transformations, kinetically stabilized versus thermally stabilized polymorphs and opportunities for control of polymorphic phase, and control of chemical processes using a variety of spectroscopic methods. Studies that yield new insights on the decomposition pathways of energetic molecules including their associated ionic states, both in the gas and condensed phases, are also of interest. The role that cations and anions play during detonation of bulk phase energetic materials is currently of high interest in the program. Proposals are especially encouraged in this area.

Research in the *Computational Modeling* thrust is focused on the development and validation of theories for describing and predicting the properties of chemical reactions and molecular phenomena in gas and condensed phases. In particular, research targeted at the development and implementation of novel theoretical computational chemistry methods is of interest. Ideally, such methods will go beyond current theories to allow for efficient, accurate, and *a priori* prediction of thermochemical properties. Such methods may take advantage of near-ideal parallel processing on massive computer clusters, or they may seek to solve current scaling problems through novel implementation of unprecedented theories via computer algorithms. The accurate prediction of intermolecular forces for problems in solid-state chemistry, such as the prediction of x-ray crystal structures, is also of interest.

Research in the *Chemistry of Novel Energetic Materials* thrust is focused on the synthesis, characterization, and measurement of properties of novel disruptive energetic materials. For a programmatic definition, disruptive energetic materials are those which have the potential to release two to ten times the explosive power of RDX when detonated. Such novel disruptive energetic materials will likely be derived from systems which differ significantly from traditional hydrogen-carbon-nitrogen-oxygen energetic materials. To be practical, any useful EM must have a high potential energy stored within the chemical bonds and also be stable from unwanted stimulations leading to accidental detonation. This principle can be used to develop notional disruptive energetic materials, and the methods of chemical synthesis can be used to target them for development. Academic research in this area is focused on discovery and characterization.

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(4) Reactive Chemical Systems

The goal of the Reactive Chemical Systems Program is to achieve a molecular level understanding of interfacial activity and dynamic nanostructured and self-assembled chemical systems to provide unprecedented hazardous materials management capabilities and soldier survivability. This Program supports basic research with Army relevance in surfaces, catalysis, organized assemblies, and stimuli-responsive chemical systems. This program is divided into two thrusts: (i) *Nanostructure Surface Interactions and Reactivity* and (ii) *Synthetic Molecular Systems*.

The *Nanostructure Surface Interactions and Reactivity* thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials.

The *Synthetic Molecular Synthesis* thrust supports research that imparts multi-functionality, stimuli-responsive and dynamic behavior to completely synthetic molecular and chemical systems. Research of interest includes design and development of nanostructured scaffolds and sequential catalytic systems. This thrust also supports research aimed at exploring the properties and capabilities of self-assembled and supramolecular structures, including their functionality, and how to control assembly in different environments.

In addition, the emerging field of dynamic, responsive, multi-functional materials have great potential to provide revolutionary new capabilities. A specific technical area in this field is "targeting and triggering" in which a specific chemical (or event) is targeted (recognized) and that recognition triggers a response. Particular technical challenges of interest include selective and reversible recognition, amplification, and multi-responsive systems. Alternative approaches to selective, yet reversible, recognition are needed.

Amplification includes an understanding of how to amplify the response from a single molecular recognition event to a multi-molecular response with approaches that promote chain reactions, self-amplification or cascade-type reactions within a single system. Multi-responsive systems in which specific stimuli trigger distinct responses are also of interest.

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(5) Environmental Chemistry

The goal of the Environmental Chemistry program is to understand the fate and transport of chemicals that in the long term will enable future force protection, situational awareness, and water treatment. This program seeks to encourage research to provide a more complete and practical understanding of chemical pathways of degradation and transformation in the environment. The research will embrace environmental complexity and heterogeneity by including the study of multiple phases and chemicals simultaneously present in an environment. Environmental surfaces of interest are soils (e.g., clay, sediments, dust), water (e.g., lacustrine, riverine, groundwater, and snow and ice structures) and films (e.g., biological and urban). The program will identify fundamental research opportunities in two main thrusts: (i) *Chemical Fate and Transport*, and (ii) *Environmental Forensics*.

The *Chemical Fate and Transport* thrust supports research that seeks to understand the mechanisms, thermodynamics and kinetics with a focus on experimental and theoretical approaches to investigate sorption/desorption, precipitation/dissolution, and (photo) degradation of chemical species under environmentally relevant conditions. Of particular interest is understanding the conditions that lead to degradation and transformation of contaminants, and develop novel speciation models of complex environmental media.

The *Environmental Forensics* thrust focuses on developing integrated experimental and computational approaches to discern chemical transformation of chemical species (e.g., contaminants) from source to point-of-detection and provide predictions of its future transformations in dynamic environments and conditions. In addition, this thrust includes research to provide information about manufacturing process and location of chemicals released into the environment.

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ii. Physics

The objective of the Physics Division is to develop forefront concepts and approaches, particularly exploiting quantum phenomena, that will in the long-term have revolutionary consequences for Army capabilities, while in the nearer-term providing for existing Army needs. In support of this goal, the interests of the Physics Division are primarily in the areas described in the following subsections.

The Division's research programs are currently focused on five research areas, including one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in physics, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Condensed Matter Physics (CMP)

The CMP Program strives to drive research that looks beyond the current understanding of natural and designed condensed matter, to lay a foundation for revolutionary technology development for next generation and future generations of warfighters.

Strong Correlations and Novel Quantum Phases of Matter. Understanding, predicting, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technology paradigms for applications ranging from information processing to sensing to novel functional materials. Interest primarily involves strong correlations of electrons, but those of other particles or excitations are not excluded. This thrust also emphasizes dynamically- stabilized electronic states and metastable phases that are not adiabatically accessible from known ground states. The program seeks to foster novel experimental and theoretical research targeting the discovery and rational design of new quantum phases of matter, along with exploring how excitations within these phases can be probed and controlled.

Topologically Non-Trivial Phases in Condensed Matter. Topologically non-trivial states of matter beyond the quantum Hall phases have shown a remarkable opportunity to advance our understanding physics as well as provide a foundation for new technologies. This thrust seeks to expand our understanding of both single-particle mean field topological states and those with strong correlations. Discovery as well as engineering of new non-trivial phases, verification of non-trivial topologies and phase transitions between trivial and non-trivial topological states and among the latter are of interest.

Unique Instrumentation Development. Advanced studies of CMP phenomena often require unique experimental techniques with tools that are not readily available. For example, unambiguous experimental verification of predicted topologically non-trivial phases can be beyond the reach of existing techniques. The construction and demonstration of new methods for probing and controlling unique quantum phenomena is of particular interest.

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(2) Quantum Information Science

Quantum mechanics provides the opportunity to perform highly non-classical operations that can result in beyond-classical capabilities in imaging, sensing and precision measurements, exponential speed-ups in computation, or networking. This program seeks to understand, control, and exploit such non- classical phenomena for revolutionary advances beyond those possible with classical systems. An overarching interest is the exploration of small systems involving small numbers of entangled particles. There are three major areas of interest (thrusts) within this program.

Foundational Quantum Physics (FQP). Experimental investigations of a fundamental nature of quantum phenomena, potentially useful for quantum information science, are of interest. Examples include coherence properties, decoherence mechanisms, decoherence mitigation, entanglement creation and measurement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. An important objective is to ascertain the limits of our ability to create, control, and utilize quantum information in multiple quantum entities in the presence of noise. Systematic materials focused research which identifies and/or mitigates decoherence mechanisms is also of interest. Models of machine learning that are based on the foundations of quantum physics are of interest. Theoretical analyses of non-classical phenomena may also be of interest if the work is strongly coupled to a specific experimental investigation, such as proof-of-concept demonstrations in atomic, molecular, and optical (AMO) as well as other systems.

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Quantum Sensing, Imaging, and Metrology (QSIM). This research area seeks to explore, develop, and demonstrate multi-particle coherent systems to enable beyond classical capabilities in imaging, sensing, and metrology. Central to this research area is the exploration of small systems involving a few entangled particles. Topics of interest in this research area include the discovery and exploration of (a) multi-particle quantum states advantageous for imaging, sensing, and metrology, (b) quantum circuits that operate on multi-particle quantum states to enable beyond- classical capabilities, and (c) methods for the readout of quantum states. Other research topics of interest are: theory to explore multi-particle quantum states useful for beyond classical capabilities, quantitative assessment of capabilities and comparison to classical systems, efficient state preparation, quantum circuits for processing these states as quantum bits, readout techniques, decoherence mitigation and error-correction for improved performance, supporting algorithms as a basis for processing circuits, connections between the solution of hard computational problems and overcoming classical limitations in imaging, sensing, and metrology, entanglement as a resource, and suitable physical systems and key demonstration experiments.

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Quantum Computation and Quantum Networking (QCON). Quantum computing and networking will entail the control and manipulation of quantum bits with high fidelity. The objective is the experimental demonstration of quantum logic performed on several quantum bits operating simultaneously, which would represent a significant advance toward that ultimate goal of beyond classical capabilities in information processing. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum computation algorithms that efficiently solve classically hard problems, and are useful for applications involving resource optimization, imaging, and the simulation of complex physical systems. Examples include machine learning, parameter estimation, constrained optimization, and quantum chemistry, among others. The ability to transmit information through quantum entanglement distributed between spatially-separated quantum entities has opened the possibility for new approaches to information processing. Exploration of quantum networking of information and distributed quantum information processing based on entanglement is of interest. These include the exploration of long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory.

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(3) Atomic and Molecular Physics (AMP)

Topics of interest within the AMP Program include (i) quantum degenerate atomic gases, both Bose and Fermi, their excitations and properties, including mixed species, mixed state, and molecular, (ii) quantum enhanced precision metrology, (iii) nonlinear atomic and molecular processes, (iv) quantum topological matter, (v) collective and many-body states of matter, and (vi) emerging areas. Cooling schemes for molecules are of importance for extending the range of systems that may be exploited. In addition, there is an interest in emerging areas of AMO physics such as states of topologically protected matter including but not limited to topological phases, emergent lattices in quantum gases, opto- mechanical interfaces, non-equilibrium many body dynamics, and many-body localization. Research efforts within the AMP Program fall within two thrust areas: *Advanced Quantum Capabilities* and *Novel Quantum Methods*. It is anticipated that research efforts within these areas will lead to applications including novel materials, efficient computational platforms, and exquisite quantum sensors.

Advanced Quantum Many-body Dynamics. The focus of this thrust is the development and study of strongly interacting many-body systems. The quantum simulator portion of the thrust seeks research on novel cooling, trapping, and the expansion of atomic and molecular species. The effort seeks the validation of many-body quantum theories through the development of experimental tools including quantum gas microscopes, synthetic gauge fields, mixed species, and novel interactions. Complimenting this effort will be the inclusion of foundational investigations into quantum mechanics, such as entanglement, many-body localization, topologically protected states, and entropy. To take advantage of the precision inherent in future quantum devices, these systems will need to connect to the classical world in such a manner that allows them to sample the signal of interest while remaining robust to noisy environments. Investigating how to maximize both the quality and quantity of entanglement within these systems will be a priority. General issues of quantum coherence, quantum interference, entanglement growth, entanglement purity, and non-equilibrium phenomena, as well as discovering new scientific opportunities are also of interest.

Novel Quantum Metrology. The AMP Program has a general interest in exploring fundamental AMP that may impact future Army capabilities. This thrust is divided into two main areas: precision metrology beyond the standard limit and harnessing collective many-body states to improve quantum sensing. The Novel Quantum Metrology efforts will expand the foundations of quantum measurement into new areas that seek to exploit entanglement, spin-squeezing, harnessing collective-spin state, developing back-action avoidance measurements, and other areas that increase fundamental precision through interactions, including cavities and Rydberg atoms. It is expected that research in this thrust will complement efforts in the *Advanced Quantum Many-body Dynamics* thrust and *vice versa*. For example, collective many body states could be studied in optical lattices or quantum gas microscopes and foundational research of entanglement and topologically protected states are anticipated to provide new metrological capabilities.

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(4) Optical Physics and Fields

The objective of this Program is to investigate physical phenomena that will lead to a deeper understanding of the underlying physics or the discovery of new physical effects that can improve capabilities of the Army. In particular, this program emphasizes physics that will significantly improve areas such as remote sensing, information processing, light and energy transmission, interactions between light and matter, and new or emerging phenomena relating to optical physics and fields. Much of the Army's capability in sensing and information and/or energy exchange depends on light. This Program also seeks research for other long-range physical fields that can complement electromagnetic radiation.

Extreme Light. This thrust focuses on research on extreme light, meaning the examination of light in the extreme limits, such as the shortest pulses attainable and the highest intensity fields attainable. Advances in these areas require theoretical and experimental research. For example, ultrashort pulsed lasers have now achieved intensities of 10^{22} W/cm^2. Future applications of these pulses may include high-harmonic generation, nanolithography, particle beam acceleration and control, and light filaments. In addition, effects such as THz formation and control and broadband localized radiation from filaments are of interest. In the near future, even higher intensities are expected. Theoretical and experimental research efforts are needed to describe and understand how matter behaves under these conditions—from single particle motion and radiation reaction to the effects in materials—and how to generate these pulses and use them effectively. Pulses as short as 80 attoseconds have been produced, and the program seeks ways to make them shorter and to understand both the physics and applications of this form of radiation. Proposals for new areas of extreme light such as relativistic optics are welcome.

Meta-Optics. This thrust pursues a fresh start in optics due to the new kinds of effects allowed by optical metamaterials. In this area, many conventional limits of optics can be broken in ways such as sub-wavelength imaging and superlensing related phenomena. It is timely to look at the quantum optics of such processes as well as research in in flat photonics. Proposals for new areas involving discrete symmetries, such as parity-time symmetries and non-Hermitian Hamiltonians are of interest. A related area is supersymmetric optics (SO), where projects are sought that use SO concepts in the design of photonic materials with nee properties or capabilities. New forms of imaging using transformation optics or other novel imaging, including quantum optics, are also of interest. In general, any optical phenomena that can ultimately improve Army capabilities are sought.

Non-Electromagnetic Fields. Other forms of propagating energy have been predicted and will theoretically have properties that differ dramatically from electromagnetism. Modern theories of gravity as well as string theory predict, in addition to gravity, the existence of two other long- range fields. If these theories are correct in their predictions, this suggests applications in which these new fields may be useful for detection or communication, especially in situations where electromagnetism and optics are not useful, such as propagating through conducting media. This program seeks proposals that may lead to the detection and/or measurement of these fields.

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iii. Life Sciences

The Life Sciences Division supports basic research to advance scientific knowledge and understanding of the fundamental properties, principles, and processes governing DNA, RNA, proteins, organelles, prokaryotes, and eukaryotes, as well as multi-species communities, biofilms, individual humans, and groups of humans. Research investments are driven by exploiting new scientific opportunities with anticipated long-term payoffs, including maintaining U.S. technological superiority and developing new Army capabilities.

The interests of the Life Sciences Division are primarily in the following areas: synthetic biology, biochemistry, neuroscience, microbiology, molecular biology, genetics, genomics, proteomics, epigenetics, systems biology, bioinformatics, and social science. The results of fundamental research supported by this Division are expected to enable the creation of new technologies for improving warfighters' physical and cognitive performance capabilities, for protecting warfighters, to create new human-machine synergistic capabilities for identifying causes of and tipping points for social/political instability, and for creating new Army capabilities in the areas of biomaterials, energy, logistics, forensics and intelligence.

The Division's research programs are currently focused on seven research areas, which includes two programs focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in life sciences, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biochemistry

This program emphasizes basic research focused on understanding and controlling the activity and assembly of biomolecules. Scientific advances supported by this program are anticipated to enable the development of novel systems, materials and processes that enhance Soldier protection and performance. An overarching goal of the program is to provide the scientific foundations to support biological activity outside of the cellular environment, including integration of biological systems with synthetic systems.

The *Biomolecular Specificity and Regulation* thrust is focused on elucidating natural mechanisms by which biomolecules recognize and interact with their targets, as well as inherent regulatory mechanisms utilized to activate or inhibit biomolecular activity. This research thrust also includes novel approaches to engineer the specificity and regulation of biomolecules, either via modulation of natural mechanisms or via design of non-natural mechanisms. The goal of this thrust is to develop novel engineered approaches to modulate and control biomolecular activity, with emphasis on achieving biomolecular control in non-cellular contexts.

The *Biomolecular Assembly and Organization* thrust is focused on understanding the molecular interactions and design rules that govern self-assembly of biomolecules into both naturally occurring biomolecular structures and non-natural human-designed architectures. Biomolecular assembly across length scales is of interest, including discrete multi-protein complexes or nucleic acid structures, as well as hierarchical protein or nucleic acid assemblies and biological composites. This thrust includes homogeneous assemblies utilizing a single building block, as well as heterogeneous systems in which a mixture of different biomolecules and/or non-biological species (e.g., minerals, synthetic polymers) assemble. This thrust aims to elucidate fundamental understanding of sequence-structure-property relationships in natural biomolecular assemblies, biomaterials, and biological composites to enable rational design of biological and hybrid biological/abiological assemblies with tailored properties and/or functions. This research thrust also includes the design of self-assembled biomolecular or hybrid biological/abiological architectures that support functional organization of biological molecules in non-cellular contexts, including artificial cells and cell-free systems, as well as novel approaches to achieve functional integration of biomolecules with non-biological materials.

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(2) Genetics

This program supports fundamental basic research in genetics, molecular biology, genomics, epigenetics, and systems biology in areas that are anticipated to enable improved cognitive and physical performance capabilities, increased survivability, and new Army capabilities in areas such as biomaterials, sensing, energy, and intelligence. This program emphasizes innovative high-risk fundamental research in areas such as identification and characterization of genetic variation, gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, epigenetics, mitochondrial regulation and biogenesis, and nuclear and mitochondrial DNA Stability and instability.

The *Eukaryotic Genetics, Genomics, Epigenetics and Molecular Biology* thrust is focused on identifying and characterizing genes, genetic pathways and genetic regulation in small and large eukaryotes. This program is interested in identifying and understanding the molecular factors and genetic polymorphisms that affect human physical and cognitive performance capabilities as well as human survival and protection under normal conditions and when affected by a variety of stressors likely to be encountered in battlefield situations, such as dehydration, heat, cold, sleep deprivation, fatigue, caloric insufficiency, pathogens, and physical and psychological stress. This program also supports pollen identification and species distribution models, mitochondrial regulation, activity and integrity, nuclear and mitochondrial DNA stability and instability, alternative animal systems, social insects, biological components of social instability, trust, plant genetics, synthetic biology, endosymbionts, and biological autonomous systems for sensing and detecting.

The *Prokaryotic Genetics, Genomics, Epigenetics and Molecular Biology* thrust is focused on understanding prokaryotic genes, genomes, molecular biology epigenetics and genetic variation. Areas of interest include mechanisms of prokaryotic adaptation at a molecular, individual and population level, prokaryotic genetic stability and instability, and synthetic biology.

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(3) Microbiology

This program supports basic research in fundamental microbiology that can help advance needs in Soldier protection and performance. There are two primary research thrusts within this program: (i) Prokaryotic Survival Mechanisms in Challenging and Extreme Environments and (ii) Analysis and Engineering of Microbial Communities.

The *Prokaryotic Survival Mechanisms in Challenging and Extreme Environments* thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie not just microbial survival in the face of environmental stress, but also the ability of specific microbes to thrive under those conditions. These stressors include extremes in temperature, pH, or salinity; the presence of toxins including metals and toxic organic molecules; oxidative stress; and cellular starvation and the depletion of specific nutrients. Included here is the study of microbial metabolism under conditions of slow growth and the transitions into and out of slow growth phases. Research approaches can include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival and environmental adaptation, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms.

The *Analysis and Engineering of Microbial Communities* thrust supports basic research that addresses the fundamental principles that drive the formation, proliferation, sustenance and robustness of microbial communities through reductionist, systems-level, ecological and evolutionary approaches. Bottom-up analysis of nutrient consumption, information exchange, signaling interactions, spatial/temporal effects structure-function relationships and biosynthetic output for single and multi-species communities within the context of planktonic and both native and engineered biofilm architectures is considered. The use of these approaches for the analysis of model microbial systems that address the biology of the mammalian microbiome are welcome. Of joint interest with the ARO Biomathematics Program, research efforts that advance the ability to work with complex biological data sets to increase understanding of microbiological systems marked by ever-increasing complexity are encouraged.

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(4) Neurophysiology of Cognition

The Neurophysiology of Cognition program supports non-medically oriented basic research in neuroscience, the behavioral sciences, physiology and neuroengineering that might enable the optimization of Soldier's cognitive and physical performance capabilities. An overarching goal of the program is to provide foundational knowledge of molecular, cellular and systems-level neural codes underlying cognition and performance across multiple length and time scales. Research in this program can include a broad range of methodological and theoretical approaches applied to animal and human experimental systems including electrophysiology, neuroimaging and computational neurobiology. This includes the study of the psycho-physiological implications of brain-machine interfaces, the measurement and modeling of individual cognitive dynamics and decision making during real-world activity, and identifying how neuronal circuits generate desirable computations. In the long term, research in this area may enable the development of interfaces enabling humans to more efficiently control machines, new training methods and devices to predict and optimize individual performance, and the potential restoration from injury at the neural level. Basic research opportunities are sought in two primary research thrusts within this program: (i) Multisensory Synthesis and (ii) Neuronal Computation.

Multisensory Synthesis. The Multisensory Synthesis thrust aims to understand how the human brain functions in relation to the interaction of sensory, cognitive and motor processes during its performance of real-world tasks. Research focuses on mapping, quantifying and modeling distributed neural processes, physiological processes and mind-body interfaces that mediate these features to ultimately develop better understanding of cognition for eventual application to Soldier performance.

Neuronal Computation. The Neuronal Computation thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Research focuses on determining how brains structure, process and refine inputs into efficient decisions and behaviors, and how these multiscale features are altered under stresses. Cell culture, brain slice and *in vivo* models are used to develop better understanding of small and large-scale living neural networks for eventual application in Army systems.

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(5) Social and Behavioral Science

The goal of this program is to promote basic research on social behavior to discover the theoretical foundations of social behavior at all levels, from single agents to collectives and global societies. The thrusts of this program are (1) developing reliable and valid measures and models of social and behavioral dynamics, (2) discovering, modeling, and validating theories of interactions among social, natural, and physical systems; and (3) generating new cross-cultural models of the impact of social institutions on the scientific enterprise.

Measuring & Modeling Social and Behavioral Dynamics. The behavior of single agents comprises a social system. The individual behaviors, however, cannot simply be summed to accurately depict or predict the dynamics of a social system. There are a number of well-documented intervening collective processes (e.g., polarization, evaluation apprehension, Ringlemann effect, risky-shift, information transfer biases, identity decay, risk transfer) that may lead to local or system-wide adjustments. Little is known about the conditions under which such collective processes are activated or how they interact to affect collective outcomes. Moreover, existing methods to detect them are often fraught with bias, relying on subjective self-reports, reliance on instruments that are not cross-culturally consistent, observer/experimenter bias, demand effects in experiments, and non-representative sampling frames. In addition to challenges in measuring social dynamics, traditional methods of modeling and empirically testing theoretical claims are often deficient. There is a tendency to use statistical techniques that rely on assumptions that are not borne out in the social phenomena being studied (e.g., assumptions of linear relationships, continuous scales, non-independence of observations, normally distributed data). The aim of this thrust is to inform and advance social science theories by generating and validate measures, methods, technologies, and models that objectively capture individual and collective dynamics to overcome this gap. The thrust looks favorably on the use of emerging methods in biophysiological measurements, measurement of social dynamics of non-human species, and cross-cultural research. It also encourages non-traditional modeling strategies that overcome deficiencies of using continuous linear models and normal distributions when phenomena are not continuous, linear, or normally distributed, as well as overcoming inappropriate assumptions of non-independence of observations. This thrust will enable new capabilities for the Army to more accurately predict risks posed by single agents, collectives, and regimes, as well as provide a foundation for understanding the basis for improving performance in and outcomes of collectives and populations.

Modeling and Validating Interactions among Social, Natural, and Physical Systems. Social systems are embedded in a larger ecological system consisting of turbulent and dynamic natural phenomena (e.g., droughts, floods, earthquakes) and constantly evolving physical systems (i.e., human-built systems, including dense urban environments, cyber environments, utility systems, transportation routes). This embeddedness imposes tensions on social systems, which may shift global social orders, impact alliances, incite conflicts, and generate sociopolitical instabilities. Different social systems, however, may be more or less resilient to the shifts in natural and physical systems. While this is anecdotally recognized, rigorous research to model the interactions among these systems is relatively new and beset with methodological challenges arising from the difficulty of tracking impacts of one system on another over different temporal and spatial expanses, the multi-level character of how effects from one system spillover to another, a lack of ability to identify how features of one system impact features of another (e.g., how the physical infrastructure of a city impacts the resilience of the city to shocks from natural disasters). Capturing the fragility/resilience of social systems to shifts in natural and physical systems will enable improved capabilities to predict emerging regions of potential future social unrest and violence, providing the Army with an early warning system to forecast and prepare for emergent conflict and the ability to plan and mobilize multidomain operations.

Modeling the Scientific Enterprise. Science is an inherently social activity and while recent research has explored the social networks of science (e.g., who publishes with whom, who mentors whom) and the demographics of actors in those networks, there is very little rigorous research on the overall enterprise of science and the impact of social institutions, like economic, political, educational, and religious systems on the trajectory of science: what leads to a discovery; how do discoveries transition to application; why do some discoveries lie dormant for decades before an application is realized, while others are almost immediately translated to application. Taxonomies related to science have been developed for example to describe (a) categories of science (e.g., Pasteur's Quadrant), (b) relations between funding and scientific activities in the research and development pathway (e.g., 6.1 – 6.7), (c) pathways from basic science to obsolescence (e.g., "cradle-to-grave"), (d) types of research strategies (e.g., "exploration vs. exploitation"),and (e) changing states of discoveries (e.g., "Sleeping Beauty Effect"). But these are merely systems of categorization and fail to capture the dynamic and socially embedded nature of science that leads to scientific discovery and leads scientific discovery to transition from one state to another. There is a long history in the philosophy of science that does recognize the social dynamics of science, but has yet to be operationalized. Organizational science has developed case studies of organizations that rapidly generate discoveries and transition them to swiftly seize market dominance. While rich in description, case studies fall short of a generalizable theory of the scientific enterprise. The aim of this thrust is to pursue new models that capture the socially embedded dynamic nature of science by focusing on science not as only a local team-driven or organizationally specific phenomena, but also investigate science as a macro institutionally motivated enterprise. A macro perspective on science will provide new insights on factors that enable both discovery and inventions that improve lives and capabilities. This thrust encourages formal modeling strategies using cross-cultural data to depict the impact of culturally unique configurations of social processes and institutions that affect science, discovery, and transitions. Success in this thrust will result in new insights on how social institutions catalyze and impede science.

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b. Engineering Sciences

Research in the Engineering Sciences is focused on basic research to discover, understand, and exploit new material systems, mechanical systems, electronics, and earth sciences that are expected to create revolutionary capabilities for the Army. Discoveries in this area are expected to lead to capabilities in materials, the sciences for propulsion, the information domain, the ballistics sciences, the protection sciences, and human sciences augmentation, well beyond the limits facing today's Army.

i. Mechanical Sciences

The Mechanical Sciences Division supports research in a broad spectrum of fundamental investigations in the disciplines of fluid dynamics, solid mechanics, complex dynamics and systems, and propulsion and energetics. Though many creative and imaginative studies concentrate on a particular sub-discipline, increasingly, new contributions arise from interdisciplinary approaches such as the coupling between aerodynamics and structures, complex dynamics and systems, combustion and fluid dynamics, or solid mechanics and structures as in the structural reliability areas. Additionally, several common themes run through much of these four sub-disciplines, for example, active controls and computational mechanics. Research in such areas is addressed within the context of the application rather than as a separate subject of study. Fluid dynamics research is primarily concerned with investigations in the areas of rotorcraft wakes, unsteady aerodynamics of dynamic stall and unsteady separation, and fundamental studies of micro adaptive flow control. Solid mechanics include a wide array of research areas such as high strain rate phenomena, penetration mechanics, heterogeneous material behavior, and reliability of structures. The complex dynamics and systems area is focused on investigations in vehicle structural dynamics, and simulation and air vehicle dynamics including rotor aeromechanics. Research in the propulsion and energetics area is concentrated on processes characteristic of reciprocating (diesel) and gas turbine engines and the combustion dynamics of propellants used for gun and missile propulsion. The following narratives describe the details of the scope and emphasis in each of these sub disciplinary areas.

The Division also supports the ARL S&T Core Technical Capabilities. This includes the Propulsion Sciences through research in hydrocarbon combustion, non-equilibrium dynamical systems, unsteady separation and dynamics stall, and vortex dominated flows S&T areas, and the Protection Sciences and Ballistics Sciences through research in energetics, multi-scale mechanics of heterogeneous solids, and low-stiffness, nonlinear materials and material systems S&T areas. These efforts also contribute to lesser extent to the Materials & Manufacturing Sciences and Human Sciences Competencies through its impacted S&T areas.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mechanical sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Fluid Dynamics

Fluid dynamics plays a critical role in many Army operational capabilities. Significant challenges exist for accurate and efficient prediction of flow physics critical for improved performance and future advanced capability. Army platforms are often dominated by flows with high degrees of unsteadiness, turbulence, multiple and widely separated spatio-temporal scales, and geometrical complexity of solid or flexible boundaries. In order to gain the necessary physical insight to enable future capabilities spanning Army vehicles, munitions, medical devices, and logistics, the Fluid Dynamics program seeks to support basic research investigations of fundamental and novel flow physics. In view of the nonlinear and high-dimensional character of the governing equations, revolutionary advances in fluid dynamics research tools are also of great interest; advanced experimental methods, sophisticated computational techniques and breakthrough theoretical advances will be critical for gaining the required fundamental understanding. There are three major subareas or thrusts within the Fluid Dynamics program: Dynamics of Unsteady and Separated Flows, Nonlinear Flow interactions and Turbulence, and Flow Stability and Control. Each of these is described in detail below.

Dynamics of Unsteady and Separated Flows. Operating conditions for many Army platforms are characterized by flows featuring unsteadiness, nonlinear interactions, turbulence, three-dimensionality and flow separation. All efforts in this thrust area will require novel and aggressive strategies for examination of the interplay between disparate spatio-temporal scales, inclusion of physically significant sources of three-dimensionality, and characterization of the role of flow instabilities and nonlinear interactions across a range of appropriate Mach and Reynolds numbers. Criteria for identifying the signature of unsteady separation and/or incipient separation are of particular interest. Historical management of physical complexity has often resulted in scientific approaches that result in the elimination of potentially critical flow physics. Research efforts that are capable of gaining deep understanding of highly complicated flows are likely to allow critical physics to be exploited, leading to significant performance gains for Army systems. As an example, shortcomings in understanding the details of unsteady flow separation, reverse flow phenomena, and dynamic stall continue to limit the capabilities of Army rotorcraft vehicle platforms. While much progress has been made towards unraveling these details, it has become apparent that revolutionary advances are unlikely if the full complexity of the physics is not considered.

Nonlinear Flow Interactions and Turbulence. As mentioned above, many Army relevant flows are governed by strong nonlinearities and turbulent behaviors. Historically, many analysis tools developed for linear dynamics have been applied to gain understanding of flow behaviors. While local insights can be gained through applications of these methods, the ability to provide global understanding of the evolution of flows requires new approaches that are capable of dealing directly with inherent nonlinearities. Operator theoretic methods show great promise in tackling the perennial difficulties associated with the Navier-Stokes equations. Turbulent dynamics may also benefit from new approaches based in dynamical systems theory to push modeling frameworks beyond the notions based on Reynolds averaging and stochastic dynamics and to determine if a useful underlying deterministic structure exists. Modeling flows near walls is a continuing challenge to accurate numerical prediction of complex physics that may benefit from novel non-intrusive diagnostics to inform creative numerical and theoretical constructs capable of efficiently producing a high degree of fidelity near physical boundaries.

Flow Stability and Control. Many of the previously described flows are susceptible to initially small amplitude, but dynamically significant, instabilities that can ultimately lead to fundamental changes in global flow behaviors. Thorough understanding and prediction of these instabilities and their growth is crucial not only to maintaining robustness in the face of disturbances, but also to gain advanced control over the evolution of flows through their exploitation. Research breakthroughs in global and local stability characteristics and their subsequent manipulation are of interest. Theoretical, computational, and experimental examinations of canonical problems to enable focused studies of interactions between instability mechanisms and global flow characteristics are highly encouraged, especially those that seek nonlinear descriptions. Flow control efforts should seek to exploit understanding of these mechanisms to permit the flow evolution to be prescribed. Flow control investigations should also seek to understand not only the impact of control actuation on the flow, but should also consider strategies for closed-loop feedback control and appropriate scaling laws that lead to the potential for such strategies to transition into new capabilities in real-world flows.

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(2) Solid Mechanics

The Solid Mechanics Program supports investigations of the behavior of material systems under extreme high loading and loading rate events, such as impact and blast, repetitive loading, temperature and pressure extremes, and prolonged operation. Development of new computational and experimental techniques and enhanced understanding of the physical processes taking place during deformation, fracture initiation, and failure are sought.

Advances in computational techniques should aim to connect phenomena occurring at different spatial and/or temporal scales, substantially improve efficiency and/or accuracy of predictions, integrate new physical relationships, apply a novel approach to studying a physical process, or expand the range of conditions at which processes can be studied. Development of experimental methods that can validate new models or visualize stress fields in complex situations are also of interest.

Maximizing strength and damage tolerance while minimizing weight and cost are key considerations for the development of new material systems; therefore, studies of all material types will be considered, and novel composites, geometries, and bioinspired structures are particularly encouraged. The effects of structure, geometry, composition, defects, and bonding across interfaces on the damage propagation across a material system are of interest.

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(3) Complex Dynamics and Systems

The Complex Dynamics and Systems program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. Further information on the current scientific thrust areas are detailed in the paragraphs that follow.

High-Dimensional Nonlinear Dynamics. Classical dynamics has produced limited fundamental insight and theoretical methods concerning strongly nonlinear, high-dimensional, dissipative, and time-varying systems. For over a century, qualitative geometric approaches in low-dimensions have dominated research in dynamics. These approaches of reduced-order-modeling of high-dimensional dynamics are often premised on empirical and statistical model fitting and are incapable of capturing the effects of slowly growing instabilities and memory. The program seeks to develop novel theoretical and experimental methods for understanding the physical and information dynamics of driven dissipative continuous systems. It also seeks novel reduced-order-modeling methodologies capable of retaining time-dependent and global nonlinearities. Novel research pertaining to the analysis and fundamental physics of time-varying nonlinear systems and transient dynamics is a high-priority.

Nonlinear Mechanical Metastructures. Another emerging area in this thrust concerns nonlinear mechanical metastructures. Emphasis is on exploiting nonlinear behavior within nonlinear mechanical lattices and lattices of nonlinear mechanical modules from the millimeter to meter scale. Proposals exploring interactions between nonlinear meta-structures with fluids, especially if such interactions augment desired dynamic behavior, are strongly encouraged.

Embodied and Distributed Control, Sensing, and Actuation. This thrust develops deeper understanding, through supporting theory and experiment, of the role of embodiment and dynamics on a physical system's capability to process information and transform energy. Proposals emphasizing the mechanics and control of soft, continuous bodies are encouraged along with novel experimental paradigms leveraging programmable printed matter. Generally, this thrust strongly leverages advances in, and approaches from, sensory biomechanics, neuromechanics, underactuated systems theory, and mechanical locomotion dynamics to understand the motion of both articulated and continuum dynamical systems operating in highly-dynamic environments. The scientific principles sought, however, are not limited to biological movement and manipulation. Proposals are strongly encouraged that view morphology in an abstract sense. For example, understanding morphology as a system's symmetry, its confinement (e.g. chemical reactions), or its coupling topology.

Statistical Physics of Control and Learning. The program seeks to lay the foundations for an algorithmic theory of control and learning that goes significantly beyond the state-of-the-art in model predictive control and integrates novel learning methodologies that are not mere variations of artificial neural networks and deep learning. Additional goals of this program is to develop an experimentally tested theoretical framework for controlling and creating new types of critical dynamics, phase transitions, and universality classes by bringing together theory and physical principles in statistical dynamics with control and dynamical systems theory (controlling statistical dynamics). Topics of interest relating to this include: nonlinear control of distributions with non-Gaussian uncertainty; non-Gaussian uncertainty representations; understanding relationships between work absorption and dynamics in the presence of fluctuations leading to emergent prediction and emergent centralization; steering multi-critical interacting dynamical systems toward desired universal scaling behaviors; externally controlling the strength of stochastic fluctuations and intrinsic noise in systems that are driven far from thermal equilibrium and display generic scale invariance; and selectively targeting and stabilizing specific self-generated spatio-temporal patterns in strongly fluctuating reaction-diffusion systems. Stochastic control at the microscale to enable novel manipulation of the dynamics of synthetic and natural biomolecular machines is also of interest.

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(4) Propulsion and Energetics
Propulsion and Energetics Research supports the Army's need for higher performance propulsion systems. Future systems must provide reduced logistics burden (lower

fuel/propellant usage) and safer (insensitive) higher energy density systems. Fundamental to this area are the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance current understanding of fundamental processes to enable truly predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes and on the peculiarities of combustion behavior in systems of Army interest.

Hydrocarbon Combustion. Research on combustion phenomena relevant to diesel cycle engines is focused on intermittent reacting flows containing fuel injection processes, jet break-up, atomization and spray dynamics, ignition, and subsequent heterogeneous flame propagation.as well. Gaining fundamental understanding of these phenomena pertaining is a major objective. Novel diagnostics for the investigation of the dense field region of the spray are of special interest. Research on heterogeneous flames requires supporting study into kinetic and fluid dynamic models, turbulent flame structure, soot formation and destruction, flame extinction, surface reactions, multiphase heat transfer, and other factors that are critical to an understanding of engine performance and efficiency. An additional consideration is the high pressure/low temperature ignition environment encountered in advanced engines, which influences liquid behavior and combustion processes at near-critical and super-critical conditions. Fundamental research is needed in many areas, including low temperature physical and chemical rate processes, combustion instability effects at low temperatures, and non-equilibrium behavior. New characterization methods to investigate kinetics and flame phenomena in-situ at high pressure are needed. New computational methods to be able to predictively model complex reacting systems are also needed. With advances in sensing, modeling, and control architectures, it is becoming possible to further optimize the performance of combustion systems. Providing the foundations for such active control is also of interest to the program.

Energetic Materials. Research on energetic material combustion processes is focused on understanding the dynamics of the planned and inadvertent ignition and subsequent combustion of these materials which are commonly used for propulsion in gun and missile systems and in ordinance. The program is also addressing the characterization of advanced energetic materials, e.g., those based on nanoscale structures and/or ingredients. Basic research is needed in several areas, including: thermal pyrolysis of basic ingredients and solid propellants; flame spreading over unburned surfaces (particularly in narrow channels); surface reaction zone structure of burning propellants; chemical kinetics and burning mechanisms; propellant flame structures; characterization of physical and chemical properties of propellants and their pyrolysis products; and coupling effects among the ignition, combustion, and mechanical deformation/fracture processes. The use of advanced combustion diagnostic techniques for reaction front measurements, flame structure characterization, and determination of reaction mechanisms is highly encouraged, especially those able to probe surface and sub-surface reactions in the condensed phase. Also of interest are novel methods which can well characterize the ignition and burning behavior of a material utilizing only minute quantities of that material. Complementary model development and numerical solution of these same ignition and combustion processes are also essential. There is also need to understand the unplanned or accidental ignition of energetic materials due to stimuli such as electrostatic discharge, impact, friction, etc. This requires, for example, research on the processes of energy absorption and energy partitioning in the materials, the effect of mechanical damage on the ignition events, and other topics relating to the safety of energetic materials.

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(5) Earth Materials and Processes

The Earth Materials and Processes program is part of an effort across both the Mechanical Sciences Division and the Chemical Sciences Division to explore areas in Earth Sciences. Specifically, the Earth Materials and Processes program seeks to elucidate the properties of natural and man-made Earth surfaces, with the goals of revealing their histories and governing dynamics and developing theory that describes physical processes responsible for shaping their features.

Earth Surface Materials aims to utilize experiments, models, and theory development to describe the physical and mechanical properties and behaviors of rocks, minerals, and soil, and to exploit the properties of these materials to provide quantitative information on recent and ongoing surface processes and perturbations.

Surface Energy Budget aims to determine, at Army-relevant spatial and temporal scales, how natural and artificial surfaces (e.g., soil, sand, or concrete) store and conduct energy depending on their spatial relationships, inherent material properties, and imparted features such as moisture storage and evapotranspiration, and to determine how these surfaces affect flows in complex terrain.

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ii. Electronics

The Electronics Division seeks to support scientific and engineering endeavors in research areas that possess the potential to define new electronic capabilities or to enhance future electronic performance. The Division is more concerned with generating basic knowledge about processes and mechanisms than creating actual devices, although prototype devices may be useful for demonstration of principle. The Electronic research sub-areas are (1) Nano and Bio- Electronics, (2) Optoelectronics, (3) Electronic Sensing, and (4) Electromagnetics and High Frequency Electronics. Proposals are sought that advance fundamental understanding of electronic and photonic processes leading to new or improved materials and devices with a strong prospect for use in future Army technology.
The Electronics Division supports many of the ARL S&T Competencies especially the Materials & Manufacturing Sciences which is supported by all Electronics' sub-areas in novel

electronic and photonic materials. The Computational Sciences Competency is supported through novel Nano, Bio, and Optoelectronic computing, Protection Sciences by active and passive sensing, Network & Information Sciences by new algorithms from biosciences as well as electromagnetic discoveries, Ballistics Sciences and Protection Sciences through targeting and directed energy, and Human Sciences through understanding and interfacing electronically with biological systems.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in electronics, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biotronics

This research area focuses on the discovery and manipulation of phenomena and the creation of new processes where electronics and biology overlap at the cellular / sub-cellular level. This length scale is where the amplitudes of many types of energies (e.g., electrostatic, mechanical, and chemical terms) converge, and correspondingly, where electronics can have fundamental biological impacts and where leveraging electronics capabilities at the nanoscale can yield unique new understanding of the cellular and intracellular processes. New electronic structures and materials are now able to focus localized static electric and magnetic fields and electromagnetic fields at the nanoscale, which presents the opportunity to selectively address and manipulate the organelles and membranes making up the structure of the cell. Moreover, cell constituents can have a frequency dependent response to mechanical and electromagnetic excitation, resulting in unique electronically enabled and controlled biological experiments. Molecular and subcellular events at the biological interfaces or surfaces are key to downstream biological dynamics. The stimulation or manipulation of these events by electronic means provides the opportunity for unique control and experimentation that are orthogonal to existing biochemical or genetic approaches. Ion flow, which is fundamental to inter- and intra-cellular signaling and process control, is susceptible to electromagnetic influence and produces electromagnetic signatures of cellular processes. The dynamics of charged and polarized cellular components also produces minute displacement currents, and can produce very large field distributions in a confined nanoscale space (e.g., within a protein scaffold or across a lipid bilayer); both of which are subject to electromagnetic probing and analysis. The different geometries of organelles within a cell result in different electromagnetic signatures and sensitivities which can be leveraged for selective control of cellular processes. Proteins play a role in almost every cellular process. As extremely large and complex molecules, they should have electromagnetic and mechanical responses that can be exploited for control. The skeletal protein assemblies of the cell, in particular, may offer a highway for the introduction of electrical currents or mechanical vibrations. Bio-chemical or genetic alteration of the interface of the cell and its components can introduce new electromagnetic properties, for example a new capability for photosynthesis in bacteria or new electromagnetic responses. Cellular engineering of membranes, cellular organelles, and proteins by the introduction of nano-particles and bio-molecules can introduce new sensitivities and new functionality. Opto-genetics is a well-established procedure for interrogating cells. Early attempts at "magneto-genetics" have been controversial, however "electro- or RF-genetics" may offer new opportunities. There may also be inherently non-trivial quantum mechanical mechanisms linked to biological behaviors, such as navigation. Inherently quantum phenomena such as the tunneling of electrons and protons play a critical role in many intracellular processes and can be modulated or manipulated with nanoscale electric fields. This research area seeks understanding and control of inter- and intra-cellular phenomena at the micro- and nano-scale.

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(2) Optoelectronics

Research in this subarea includes novel semiconductor structures, processing techniques, and integrated optical components. The generation, guidance and control of UV through infrared signals in semiconductor, dielectric, and metallic materials are of interest. The Army has semiconductor laser research opportunities based on low dimensional semiconductor structures (quantum dots, wells, wires, etc.) operating in the eye-safe (>1.55), 3-5, 8-12, and 18-24 microns regions for various applications, such as ladar, infrared countermeasures, and free space/integrated data links. Components and sources in the UV/visible spectral ranges (particularly < 300 nm) may be of interest as well. Research is necessary in semiconductor materials growth and device processing to improve the efficiency and reliability of the output of devices at these wavelengths.

Research that leads to an increase in the data rate of optoelectronic structures is sought. Interfacing of optoelectronic devices with electronic processors will be investigated for full utilization of available bandwidth. Electro-optic components will be studied for use in guided wave data links for interconnections and optoelectronic integration, all requirements for high speed full situational awareness. Optical interconnect components are needed in guided-wave data links for computer interconnection and in free-space links for optical switching and processing. For high-speed optical signal processing as well as potential for power scaling, research on individual and 1 or 2-D arrays of surface or edge-emitting lasers is necessary. Research addressing efficient, novel optical components for high speed switching based on plasmonics, quantum dots, metamaterials or other regimes may be of interest. Emitters and architectures for novel display and processing of battlefield imagery are important.

Recent advances in neuromorphic photonic information processing (neurophotonics for short) and computation are highlighted a thrust of interest. Neurophotonic processing within a photonic IC (PIC) requires smaller and more energy efficient modulator devices on the order of 5 microns or less and 1 femtojoule/bit. Speeds of modulation should be several Gb/s or higher, and the insertion loss should be < 0.1 dB to achieve cascaded modulators of < 1 dB/cm. Modulation at 16 bit or higher resolution will be required for neurophotonic processor implementations. Other advances leading to enhanced neurophotonic regimes including energy efficient and high-speed photodetectors and light sources (most likely coherent) are sought. Exploration of ideas leading to enhanced performance in both 2D and 3D architectures that take advantage of bosonic properties of light (over the limited fermionic charge) will be considered. While single photon, quantum communications and quantum integrated photonics are not focused upon here, low photon (<100) count signals can be considered. Such research could impact single photon regime work with overlap due to similar quantum optics considerations.

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(3) Electronic Sensing

The ultimate goal of Army sensing is 100% situational awareness to include day/night, all weather, non-line-of-sight and through natural and man-made obstructions for sensing of vehicles, personnel, weapons, chemical and biological threats, projectiles, explosives, landmines, improvised explosive devices (IEDs), and motion. Novel techniques that enhance the stimulus-response characteristics of nano-structures and semiconductor devices are of interest. This includes ways to improve the absorption of the signal, conversion (transduction) of the signal to another form with higher efficiency, and techniques to lower the noise. Sensing technologies of interest to this research sub- area currently include acoustic; seismic; passive electromagnetic; magnetic, and light-matter interactions. Other technologies that meet an Army need are also welcome, however chemical, biological, and radar sensing techniques are generally funded through other sub-areas as is image processing.

Light-matter interactions at infrared and ultra-violet wavelengths are of particular interest. Efforts are sought that improve the quantum efficiency and lower the noise such that the signal to noise ratio is maintained as the temperature is increased. Research opportunities include components based on quantum confined devices and semiconductor materials operating in the infrared 1-24 microns regions as well as the ultra-violet spectral region. In both regions, fundamental studies involving growth, defects, interfaces, substrates, doping, and other electronic characteristics will be considered. Back-of-the-envelope calculations of the detectivity or noise equivalent power should be included for proposals involving infrared and ultra-violet detection.

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(4) Solid State and Electromagnetics

This research area emphasizes efforts to discover and create unique electromagnetic phenomena in solid-state materials and structures. Innovative research is sought in areas involving quantum phenomena, internally and externally induced stimulus, and novel transport and electromagnetic interaction effects in solid-state electronic structures. This basic research will address issues related to design, modeling, fabrication, testing and characterization to include the ability to individually address, control, and modify structures, materials and devices, and the assembly of such structures with atomic-scale control into systems. It will seek to realize advanced device concepts with revolutionary capabilities.

This program will explore the latest developments in semiconductor materials and device physics, such as negative capacitance transistors, tunneling field effect transistors and ultra-wide bandgap materials. More importantly, it will emphasize scientific discoveries in the frontier of nanoelectronic materials and structures. Scientific opportunities in this research include, but are not limited to, quantum-confined structures (nano-tubes/-wires/-dots) and large- scale precise alignment and integration of these structures to create collective behaviors; 2D atomic crystals and their heterostructures; complex heterostructures of 2D crystals, topological insulators, Dirac and Wely semimetals and other dissimilar nanoelectronic materials potentially leading to unique interfacial phenomena; spintronic, valleytronic, and mixed domain (charge/spin/quantum degrees of freedom) device concepts. Of interest are quantum transport phenomena such as ballistic transport and hydrodynamic flow, dissipationless transport in topologically protected edge states, and pseudo-relativistic transport of massless Dirac fermions. Exotic electromagnetic phenomena which require theoretical formulations beyond the well-established Maxwell's equations, such as axion electrodynamics, chiral anomaly and spontaneous symmetry breaking, are also relevant. Interfacial proximity effects in these heterostructures that lead to unique electromagnetic properties will also be considered.

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iii. Materials Sciences

The Materials Science Division of the ARO seeks to realize unprecedented material properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army with special emphasis on: Materials Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. Research supported by the Division seeks to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. The work, although basic in nature, is focused on developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multi-component and complex materials is of particular interest. Foundational research that integrates novel experimental work with the development of new predictive materials theory is also of significant interest. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in materials science that may have future applications for the Army.

The Division supports the ARL Materials & Manufacturing Sciences Competency by aggressively seeking to extend the state-of-the-art in materials design, mechanical behavior of materials, physical properties of materials, and synthesis and processing research. It further accomplishes this with unique materials for advanced power storage and generation and lightweight structures, in addition to low-cost manufacturing and repair processes. It supports the ARL Ballistics Sciences with extraordinary lightweight materials, force-activated materials, stabilized nanostructured materials, manufacturing process science, novel electronics, and advanced sensory materials. It also supports the ARL Computational Sciences with research efforts that integrate computational theory and precision experimental measurement to design and optimize advanced materials.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in materials science, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Materials Design

The Materials Design program supports experimental, theoretical, and computational studies that design, create, and understand novel functional materials from the bottom-up. The foundations established here support the realization of advanced "smart materials" concepts like reconfigurable optics and electronics, bio-mimetic materials, and multi-functional materials that dynamically respond to their environment.

The Science of Self-Assembly supports basic research into the multiple physical and chemical forces at play during directed, bottom-up 3-D assembly into super-structures incorporating multiple components. This knowledge can be used to design novel self-assembled materials that would be impossible to create using top-down techniques. Self-assembling materials systems of interest include: soft materials like polymers; particulate systems like colloids; porous materials like gels; semiconductor nanostructures; and/or hybrids of these materials.

Reconfigurable and Hierarchical Materials supports the design and synthesis of materials that can reversibly change their properties, as well as hierarchically structured materials with emergent behavior. Areas of interest include: bio-mimetic materials; metamaterials and metasurfaces; and materials systems that undergo reversible transformations accompanied by dynamic property contrast.

Computer-aided Materials Design seeks to leverage recent advances in machine learning, artificial intelligence, computational materials science, and other numerical approaches to solve difficult materials design problems, particularly those in self-assembly and reconfigurable materials. Points of interest include inverse design of self-assembled materials; data-driven design of heterogeneous hierarchical materials; and novel models or algorithms for solving materials-specific problems.

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(2) Mechanical Behavior of Materials

This program focuses on basic research investigations that enable unprecedented mechanical behavior across a broad spectrum of advanced structural materials in order to ensure high performance under a variety of extreme and highly variable operational conditions. Experimental, theoretical, and numerical efforts are encouraged, particularly those that promote understanding of the underlying physical mechanisms leading to extraordinary behaviors. Studies may focus on a variety of materials, including: metals, ceramics, polymers, composites, and hybrid structures. Research efforts that leverage recent discoveries in other scientific fields, such as Physics, Chemistry, Biology, and Data Science, are also highly encouraged. These investigations are expected to enable transformative capabilities for the Soldier in the areas of protection, maneuver, and sustainability. Current focus areas for this portfolio include, but are not limited to, the following:

Extreme Mechanical Behaviors. This thrust emphasizes novel concepts that enable materials with dramatic improvements in the state-of-the-art for mechanical behavior, including: energy dissipation, toughness, stiffness, hardness, and resiliency. Areas of interest include new understanding, control, or confinement of deformation mechanisms; exploiting heterogeneous material systems and interface/interphase interactions to enable unprecedented properties while avoiding inherent sub-system weaknesses; and novel approaches for materials to perform in extreme thermomechanical environments.

Active Mechanical Response. This thrust focuses on structural materials that actively respond to dynamic loading environments and other external stimuli through rapid adaptation of shape, topology, or mechanical properties. Areas of interest include mitigation or manipulation of stress wave propagation; novel actuation schemes that generate extraordinary forces or that require minimal input energies; and novel material responses initiated through multiaxial loading.

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(3) Physical Properties of Materials

The Physical Properties of Materials program seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic/optical, magnetic and thermal properties in advanced materials to enable innovative future Army applications.

Novel Functional Materials supports the discovery of novel functional materials such as oxide super-lattices, nitrides, free-standing 2D materials, heterostructures, organic-inorganic hybrids, Spin-Caloritronic materials, co-crystals, and other such materials with unique structures/compositions. The thrust focus is on the synthesis, modeling and novel characterization of these materials (organic/inorganic/hybrids) to determine unprecedented functional properties (semiconducting, superconducting, ferroelectric/multiferroic, photonic, magnetic, thermal etc.).

Science & Engineering of Crystal Imperfections explores the influence (either positive or negative) of various crystal imperfections (e.g. point, line, area, volume defects etc.) on the physical properties of functional materials, and elucidates different mechanisms of incorporation of these defects during thin film growth/bulk materials processing of materials to influence the resulting extraordinary functional properties.

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(4) Synthesis and Processing of Materials

The Synthesis and Processing of Materials program seeks to discover and illuminate the governing processing-microstructure-property relationships to enable optimal design and fabrication of nano or micro structural bulk structural materials.

Processing Induced Material Design supports research focused on innovative processing methods capable of fabricating materials with deliberate microstructural architectures and features that advance the material's properties to levels unattainable by conventional processing.

Manufacturing Process Science supports investigation into fundamental physical laws and the unique phenomena occurring under metastable and far-from-equilibrium conditions to develop revolutionary and disruptive new materials or processing methodologies.

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(5) Innovations in Materials (International Program)

As one of the ARO International Programs, the Innovations in Materials Program is focused on supporting research at institutions outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which future material technologies depend.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

iv. Earth Sciences

The Earth Sciences effort of the ARO seeks to advance understanding of the terrestrial environment for the U.S. Army with special emphasis on Earth Materials and Processes and Environmental Chemistry. Research is cooperatively managed by the Chemical Sciences Division (managing the Environmental Chemistry Program) and the Mechanical Sciences Division (managing the Earth Materials and Processes Program). Together these efforts seek to explore the properties of Earth materials and chemical species to discover how they interact with their environments and respond to external forces. Knowledge of the fundamental properties of these materials, from the atomistic to the landscape scale, and their interactions with the atmosphere, hydrosphere, and biosphere are relevant to Army operations, infrastructure, and stewardship. Fundamental research lays the foundation to support a range of Army needs, including the remote characterization of land surfaces, trafficability of ground vehicles, and environmental priorities such as waste management and remediation. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in Earth science that may have future applications for the Army.

Detailed descriptions of the two programs can be found under the respective managing divisions. Earth Materials and Processes Program in Mechanical Sciences and Environmental Chemistry in Chemical Sciences.

c. Information Sciences

Research in the Information Sciences is focused on discovering, understanding, and exploiting the mathematical, computational, and algorithmic foundations that are expected to create revolutionary capabilities for the future Army. Discoveries in this area are expected to lead to capabilities in materials, the information domain, and Soldier performance augmentation, well beyond the limits facing today's Army.

i. Computing Sciences

The principal objective of the ARO Computing Science Division is to provide increased performance and capability for processing signals and data, and to extract critical information and actionable intelligence to enhance the warfighters' situation awareness, decision making, command and control, and weapons systems performance. The Division supports research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and theories governing intelligent and trusted computing. More specifically, the Division aims to promote basic research to establish new computing architectures and models for intelligent computing, create novel data fusion and extraction techniques for efficient information processing, and build resilient computing systems for mission assurance. The results of these research efforts will stimulate future research and help to keep the U.S. at the forefront in computing sciences. The research topics described in this section of the BAA are those needed to provide the warfighters with the latest information science and technology to achieve the vision of future Army operations.

Research in the Computing Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Network & Information Sciences Competency goal of algorithm design for object classification and scene understanding from active and passive 3D scenes and full motion video through enhanced semantic object recognition; (ii) Computational Sciences goal of large scale computing and modeling, and dynamic multi-dimensional heterogeneous data analytics, by devising scalable algorithms that effectively handle the size, complexity, heterogeneity, and multi-modality of data and by creating new hardware and software architectures for emerging and future computing systems that optimize the use of Army computational resources; and (iii) the Network & Information Sciences Competency goal of estimating adversarial dynamics and infrastructure through new game models for capturing attacker/defender interactions and better predication of adversarial mental state (intent, capability, and decision process) to enable better cyber defense.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in computing science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Computational Architectures and Visualization

The Computational Architectures and Visualization program is concerned with modeling, analysis, design, and validation of computational infrastructure, both hardware and software, with special emphasis on the effect emerging and future computational architectures will have on managing, processing, analyzing, and visualizing massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, analyze, and visualize such massive amounts of information. Emerging architectures only exacerbate the problem because the present and traditional models of computation no longer apply.

The research strategy is to focus on the effect that the technological shift to these new, advanced architectures will have on newly-developed systems and how to compute with these architectures efficiently as well as to make very large simulations and the visualization of massive data sets more interactive for the user while maintaining a high level of accuracy. As such, this programs funds innovative architectural designs of both hardware and software components and their interfaces that efficiently optimize computational resources and innovative algorithms that render massive data sets and/or massive geometric models and perform large scale Army simulations both quickly and accurately. Advances in this program are expected to lead to new computer modeling and design concepts (or paradigms) as well as software libraries that compute efficiently on these new and emerging architectures, that are scalable (usable on large-scale complex problems and able to handle massive amounts of data), and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. Also to be expected is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

Computational Architectures. Future computer systems will be both massively heterogeneous and parallel, implying the present and traditional models of computation will no longer be applicable. As a result, new computational theories are needed as well as mathematical abstractions and models of computation to address the difficulties associated with heterogeneous, parallel and distributed processing. Of special interest is determining how these new abstractions, algorithms, and computational processes map onto emerging computational resources of different types (e.g., multi-core, quantum, cloud, and chaotic computing, and determining which platforms are most suitable for

Army applications). Other important issues to be considered for these emerging and future architectures are programmability, language and compiler support, real-time scheduling, resource-allocation, and the development of a flexible software environment.

Visualization. Interactive simulation and visualization provides new and enhanced capabilities for the examination, exploration, and analysis of information and data critical to the Army. However, Army applications are not limited to any one type of data or computational platform. As a result, new research and techniques are needed in order to visualize and simulate complex Army data such as training for battlefield scenarios with speed and precision on any platform for superior analysis and information extraction capabilities for realistic Army simulations and full situational awareness. Specific research areas of interest are, but not limited to, computational geometry, robust geometric computing, geometric and solid modeling, interactive graphics, 3D visualization tools, verification and validation, and synthetic environments. Special emphasis is placed on making very large simulations and the visualization of massive data sets faster, more computationally efficient, and more interactive for the user while maintaining an appropriate level of fidelity and physical realism.

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(2) Information Processing & Fusion

With ubiquitous data acquisition capabilities, effective data and information processing is of critical importance to defense missions. The Information Processing and Fusion program is concerned with the creation of innovative theories and algorithms for extracting actionable intelligence from diverse, distributed multimodal data to support Army operations.

Foundations of Image and Multimodal Data Analysis. Innovative research is sought concerning: (1) novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information, with particular emphasis on data in complex forms such as image or video data; (2) detection, localization, and recognition of objects and locations from image data with particular emphasis on provable performance guarantees; (3) detection of events, actions, and activities to extract activity-based intelligence, especially when no extensive training data is available; and (4) integrated approaches that enable semantic descriptions of objects and events including relations. Learning and adaptation should enable the representation at both low and high-levels, where inputs from actual users of the systems are used to improve the performance of the algorithms and the fidelity of models at all levels of the modeling hierarchy. Also of interest are methods to exploit the structure of the data, capture its intrinsic dimensionality, and extract information content of data. The development of an "information/complexity theory" and a "learning theory" specific for remote sensing, imaging data, and decision tasks is highly desirable.

Data and Information Fusion. Multimodal data acquisition systems are increasingly prevalent with disparate sensors and other information sources. This thrust seeks advanced mathematical theories and approaches for integrating multimodal data and contextual information to provide actionable intelligence. Of particular interest are systematic and unifying approaches for data and information fusion from diverse sources. Scalable methods are needed for efficiently handling vast amounts of data. Fusion in networked environments addressing issues such as adaptive, distributed, and cooperative fusion is emphasized. Theories and principles for performance analysis and guarantees at all fusion levels to support robust data and information fusion are important to ensure successful military operations.

Active and Collaborative Sensing. Modern sensing systems typically include multiple networked sensors with communication capabilities where the whole network can be thought of as a Meta sensor that can be controlled, in addition to each individual node having some controllable degrees of freedom such as mobility for unmanned aerial/ground systems, pan-tilt-zoom for infrastructure sensors, or waveform for agile radar. Depending on the task or query, it is desirable for the system to control the data acquisition process so as to acquire the "most informative data" for the specific task or query. Consequently, of particular interest are methods that address the integration of mobility, sensor-selection, modality selection, and active observation for real-time assessment and improvements of sensing performance. Another research area of interest is performance-driven active data collection. A query is given to the system together with a desired performance bound. Where the confidence in answering the query is insufficient, the system should actively interrogate or control sensors in order to achieve the desired confidence. Such an active learning and information-driven sensor control should include the Soldier in the feedback loop.

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(3) Intelligent Information Systems

The overall objective of the Intelligent Information Systems program is to augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats which is in line with the DoD's adoption of net-centric warfare, variously defined as flattening the information space to interconnect Soldiers and commanders to provide instantaneous access to information, knowledge, and situational awareness. Given this goal, it becomes necessary to understand (a) fundamentals of what intelligence means in the context of autonomous systems and how to build intelligent systems especially as it relates to interaction amongst a network of humans and machines, and (b) foundational algorithmic issues in representation and reasoning about networks inherent in societies and nature.

Information Networks. In order to model network effects it is necessary to algorithmically represent large networks and reason about them. Unfortunately, information about networks is seldom complete – data available might be missing crucial pieces of information, might have contradictory pieces of information, or could be approximate (with associated notions of uncertainty). Representing and reasoning about these networks requires advances in knowledge representation, graph and data mining, natural language processing, algorithmic graph theory, machine learning, and uncertainty quantification and reasoning. Examples include the emerging area of Graphons which provide new tools for generating and reasoning about graphs that occur in practice (satisfying power law distributions), but also provide new tools for Machine Learning. In particular, a major goal of this thrust are tools and techniques that allow data driven approaches to capturing latent relationships with powers to both explain and predict. Advances in this thrust would not only lead to improved autonomous systems and algorithms, but also enhanced-embedded battlefield intelligence with tools for creating necessary situational awareness, reconnaissance, and decision making. Finally, it should be noted that algorithmic notions of approximations, tight performance bounds, probabilistic guarantees, etc., would be major concerns of the solution space.

Adversarial Reasoning. Development of appropriate mathematical tools to model and reason about societies and cultures, that brings together tools from Game Theory, Social Sciences and Knowledge Representation. Research of interest includes, but is not limited to, Game Theory for security applications while accounting for bounded rationality, development of Game Theory based on data regarding cultural and adversarial groups, and Behavioral Game Theory that can explain intelligence in groups and societies. In particular, the role of human biases in decision making and game theory is of importance to this thrust of the program.

Natural Language Processing and Affective Computing. Inference algorithms work incredibly well when data is in a structured format. However, most reports, email, and conversations are written out as text with information embedded in them. This thrust seeks advances in purposeful Natural Language Processing at scale that can account for context and mode-switches by bringing together statistical and logical methods. Indeed, when combined with other signals, such as video signals, the inter-play of non-verbal and verbal/ textual communication provides rich contextual information, which, in turn, leads to accurate information being gleaned from an interaction.

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(4) Advanced Learning

Advanced Learning, including both embodied systems and software agents, play an increasingly important role in civilian and military settings. With few exceptions, current intelligent systems are restricted to highly constrained environments for short duration missions. Future systems will need to perform a variety of tasks in complex, possibly contested, open worlds for extended periods of time. One important characteristic of open worlds is that the intelligent system will encounter new contexts, activities, and objects that will require it to adapt previously trained algorithms. Advanced capabilities in learning, knowledge representation and reasoning, interaction, and assured operations are essential to the development of intelligent systems that can greatly enhance the Army's mobility, agility, lethality, and survivability in future conflicts.

Learning Theory, Methodology, and Techniques. Over the past 50 years, machine learning has made great strides in classification, natural language processing, and task learning. However, machine learning still lacks the rigor, agility, and flexibility necessary to operate in complex, contested open worlds. This thrust focuses on establishing a theoretical foundation for on-line or continuous machine learning. New learning approaches will need to address both the dimensionality challenges and temporal characteristics that may be evolving continuously. In addition, new techniques must address robustness to enable the learning system to deal with novelty, noise, observation errors, and potentially malicious input that aims to disrupt learning. Innovative approaches to continuous learning will allow systems to adapt to changing contexts and environments while maintaining previously learned knowledge. Under this thrust, we investigate approaches that help the intelligent systems deal with dynamic environments, devise new, transferable skills, and cope with unknown situations. Skill acquisition focuses on developing new theories for learning, creating, and combining low-level skills into more sophisticated behaviors.

Knowledge Representation, Reasoning and Decision Making. Long duration autonomy requires intelligent systems to manage information from different sources, including humans, knowledge bases, and external and on-board sensors. Data collected at different times and locations needs to be fused into a consistent understanding of objects and events in the environment, to support decision making and efficient communication with humans or other entities. Long duration autonomy requires reflecting on past experiences, combining, comparing, and using those experiences in new contexts to make decisions. Innovative research in representation and reasoning will enable future intelligent systems to manage information in both short and long-term memory systems, and develop new information through reflection and learning. Concepts from cognitive science may impact both the representation and storage of information and the ability to quickly retrieve pertinent information. New approaches are needed to address potential issues with learning systems such as, catastrophic forgetting, lack of storage capacity, and development of to external knowledge stores.

Interaction. Future autonomous systems must interact physically with humans and other intelligent systems operating in the same space, remotely with spatially distant entities, and virtually in cyberspace with intelligent software agents. New research in human-robot interaction and robot-robot teaming will enable humans and robots to share the same space and work together on complex tasks. Advanced concepts for networks of intelligent agents will enable robots at the tactical edge to draw upon off-board resources such as, software agents, humans, or other robots to solve local problems as well as contribute to a shared knowledge base, and coordinate and collaborate with others for larger problems in dynamic environments. New research in game theory, deception, and other approaches will enable intelligent systems to operate effectively in a contested environment. Future battlefields pose a number of challenges in communications including, limited bandwidth and the availability of secure communication channels. New concepts are needed to build and maintain shared, but possibly distributed, information models for these environments.

Assured Operations. Test, Evaluation, and Verification and Validation for intelligent systems is a nascent field that needs rigorous theoretical underpinnings and practical tools. Long duration missions require intelligent systems that can operate safely and reliably in an open world environment. Extending techniques from computer science and control theory, such as control barrier functions and model checking, can help ensure safe operations during both learning and execution of mission-related activities, but these techniques by themselves are not sufficient for assured operations. Theoretical advances in architectures, control theory, and introspection are needed to enable systems to adapt to temporary or permanent changes to internal and external conditions in a timely manner. Advances in risk-aware online planning will enable autonomous systems to balance conflicting objectives and operate safely in poorly understood environments.

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ii. Mathematical Sciences

The objective of the Mathematical Sciences Division is to support research to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models.

Research in the Mathematical Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Information Sciences Competency goal of image and video sampling and reconstruction through investigations of sparsity in combinations of distributions with unknown parameters; (ii) Computational Sciences Competency goals of stochastic simulation methods, interfaces and evolving topologies, and uncertainty propagation, through investigations of fast separable methods for stochastic PDEs, of novel meshes for both front tracking and domain-fitting, and of weak-interaction processes; (iii) Computational Sciences Competency goals of computational social sciences by establishing a general theory of crisis/change through new mathematical models that go beyond network models to incorporate morphisms as model elements; (iv) Human Sciences Competency goals of brain networks and of cognitive and neural modeling, through investigations of neural dynamic models and their computation; and (v) Computational Sciences Competency goals of stochastic optimization and modeling through investigations of fast separable methods for stochastic PDEs.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mathematical science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Modeling of Complex Systems

The Modeling of Complex Systems Program is a program of fundamental mathematics oriented research, the broad objectives of which are twofold. First, the program seeks to develop and analyze new, innovative, and robust modeling frameworks that may be adapted and generally applied across a variety of disciplines. The second goal is to develop both quantitative and qualitative models of specific complex phenomena in areas in which current models are either not fully based on first/basic principles or are based on empirical and ad hoc metrics for which the first/basic principles are not yet well known. Although they break down into more specific research directions, the three thrust areas of interest to the Modeling of Complex Systems Program are 1) development and analysis of new, general modeling frameworks, 2) geometric and topological modeling – which can be further broken down into more specific thrust areas, as noted below – and 3) small and large group social modeling and social informatics.

Metrics – in the general, non-mathematical sense of the word – are a natural part of the mathematical modeling framework. Traditional metrics, when they exist, often do not measure the characteristics in which observers in general and the Army in particular are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. As is the case for the modeling effort, these metrics should preferably be in a complete mathematical analytical framework, which is to say, in part, that they should derive from the problem in question as opposed to a situation in which one forces the model to fit an *a priori* chosen metric. The research in modeling of complex phenomena supported by the Modeling of Complex Systems Program is primarily mathematical analysis and *not* numerical analysis or computational mathematics. One expects computation to play some role in any modeling endeavor, but the innovation in research carried out in the Modeling of Complex Systems program should be largely in the areas of modeling and analysis, and not in the computational techniques.

Furthermore, any modeling research effort that could be of benefit to military or intelligence applications but that might not fall directly under one or more of the program thrust areas will still be considered, particularly if the innovation in the modeling and analysis are significant and noteworthy.

The three major areas of research of the Modeling of Complex Systems Program are:

Modeling Frameworks and Analysis. Mathematical and physical modeling is fundamental to nearly every other direction of research in the physical, social, and computational sciences. A common element of modeling – even if the phenomenon in question is highly complex – is to incorporate simplifying assumptions that sacrifice realistic application and utility for computational ability. For Army and DoD applications, however, such simplifications often render the model impractical. Modeling frameworks are desired that are able to eschew the usual computational simplification assumptions and realistically capture, adequately govern and/or control, and effectively operate within the particular complexities of real world environments and phenomena, while still maintaining some degree of computational tractability. Of specific interest are causal and predictive modeling frameworks, hybrid model frameworks that capture both causal and predictive features, statistical modeling frameworks, and abstract categorical models (cf. Homotopy Type Theory).

Models of particular complex systems that address and are to be utilized for more specific purposes and objectives will be assessed within the context of one of the program's other modeling thrust areas described below. Research carried out under this section should address the general theory and analysis of mathematical modeling from a broader perspective.

Geometric and Topological Modeling. Representation of complex, irregular geometric objects and complicated, often high-dimensional, abstract phenomena, functions, and processes is fundamental for Army, DoD, and civilian needs. Such needs arise in the modeling of urban and natural terrain, geophysical features, biological objects (e.g. human brain mapping), information flow, and many other contexts. Any research that incorporates an innovative geometric and/or topological approach to address a problem with military, defense, and intelligence applications is welcome and will be considered, but there are two specific threads that are of particular interest to this thrust of the program: 1) geometric data analysis, and 2) multiscale geometric modeling, including dynamics and physical modeling on domains with fine, complex, geometric and/or topological structure.

Geometric data analysis includes – among other subfields – topological data analysis, subspace analysis, principal component analysis, and dimension reduction techniques. Current research directions of importance to Army applications include video, audio, and image processing (i.e. mathematical signal analysis), fast and accurate face/object recognition (i.e. reconstructing and matching geometric data through queries over a database), geometrically motivated methods and structures for working effectively with large – and often real-time extracted – data sets that may be corrupted in some way (e.g. missing or distorted data), and the application of persistent homology in the detection and classification of signals by shape. For instance, although good progress has been made in this direction, real-time capture, representation, and visual reproduction of 3D terrain – not just as a height field but with multivalent height functions and clearly defined topological obstructions – obtained directly from real-time or stored point-cloud data cannot be fully achieved with current techniques like the multitude of variations of piecewise planar surfaces that are presently studied. New approximation theory that does not require the classical assumptions – primarily smoothness – and that provides structure for the many new non-smooth approximation techniques currently under investigation is required. Concurrently, research on the metrics by which we measure and evaluate the approximation is needed.

Additionally, approximation theory for information flow and other abstract phenomena in large wireless communication, sensor and social networks is also of interest. The approximation theory developed under support of this program is expected to provide building blocks for computational geometry, pattern recognition, automatic target recognition, visualization systems, information processing and network information flow.

Multiscale geometric modeling, analysis, and dynamics are of particular interest, both in the context of models of physical phenomena over real-world terrain and in the aforementioned complex, high-dimensional data structures. Models that make use of self-similar structures and recursively defined spaces (e.g. fractals, solenoids, etc.) would be of great interest in adapting or enhancing current techniques in areas such as data mining, fluid and heat flow, and search, evasion, deployment, and maneuver over complex terrain that exhibits self-similar properties (e.g. urban or mountainous terrain). Current techniques for dealing with complex dynamical processes and large, noisy, and possibly corrupted data sets could be greatly improved in both the time and efficiency realms by employing techniques from scale symmetry, which often allows one to reduce a large and unwieldy number of variables to a more manageable problem if the variables are appropriately scaled. Models that adapt self-similarity and automata theory, in particular, can oftentimes lead to mapping complex dynamical systems problems into an algebraic and/or topological category, which then may allow for entirely new tools and approaches to be used. Homotopy Type Theory and its applications are such an area that is of significant interest in military applications.

Small and Large Group Social Modeling. Both qualitative and quantitative analytical models of social group dynamics and information flow are required for operations, training, simulation (computer generated forces) and mission planning, as well as real-time analysis, processing, and dissemination of information. Current models have limited accuracy. Research focused on mathematically justified, practically useful, computationally tractable and data-tractable models is needed. ("Data-tractable" means "does not require more data or more detailed data than is realistically likely to be available."). Research on the metrics in which the accuracy of the models should be measured is also vitally important.

The broad term for this research pursuit would be social informatics, which is an important area in which more significant progress is needed, especially in the military and intelligence realms. Social informatics, briefly, is the study of the role played in society by information-based technology. This includes examinations of how the spread of information through technology effects social and organizational changes in society, as well as the converse – how social organization of information and use of technology to spread information are affected by social structures and practices. Modeling of the flow, dissemination, and possible evolution of belief systems and cultural factors through physical group migration or through social networking is an important tool in being able to predict where social and military issues might arise in the world. This could lead to better preparation and the avoidance of "caught-off-guard" situations in global politics and military affairs.

Included within the social informatics realm are narrower but equally important research directions. These would include – but not be limited to – the dynamics of information flow across physical groups of people as well as social/technological networks, pattern detection in information flow and language, which would lead to more efficient surveillance and pre-emptive threat detection, as well as security in information transmission. In this latter direction, new and unique data structures and encryption techniques would be hugely beneficial. Complex but tractable multiscale data structures and viable fractal or self-similar encryption techniques – which heretofore have proved to be of academic but not very practical interest – are just a few examples of many that could prove useful.

Paralleling the pursuit of social informatics, information flow analysis, and pattern recognition in information and data is the quickly developing field of deep machine learning. The Army is particularly interested in developing programming models and training algorithms that can automate as much of these processes as possible. This involves a great deal of research into pattern recognition and data analysis, as well as model analysis. The interplay between causal, data-based models and predictive modeling are of special interest and an active area of military research.

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(2) Probability and Statistics

The Probability and Statistics (P&S) program accepts proposals in all areas of probability and statistics that may aid in the development of new Army capabilities. The program emphasizes two main thrust areas, of which the first thrust area is in the foundations of statistics. Recent developments, such as the rise of data science and machine learning, and the reproducibility and replicability crises have led to renewed interest in the foundations of statistics. Since the Army is a major consumer of statistical analyses, it is naturally interested in their foundations. The P&S program will concentrate on foundational issues that are still unsettled but not adequately supported by other funding agencies. The second thrust area is in developing statistical methods for data types that are of special interest to the Army.

Foundations of Statistics. This thrust is divided into two major topics. The first is near-optimization. Many statistical and decision problems are framed as optimization. That is, we write down a set of equations that describe the system we're studying, and then we look for the optimal point, or a nearly optimal point, in the space of inputs. However, in many problems it would be better, for reasons of robustness, interpretability, and implementation among others, to find the entire region of the input space that is nearly optimal. The near-optimization topic seeks proposals that will develop methods for finding, at least approximately, that region of the input space.

The second major topic addresses the possibility that there may be many good statistical models of the same data. Many statistical data analyses proceed by positing a statistical model – e.g. linear regression with Gaussian errors -- checking that the model describes the data reasonably well, then fitting the model. But it's possible that, for example, a generalized linear model or a treed regression would also describe the data reasonably well. The many-models topic seeks proposals for research that will help identify cases when many different models all describe the data well, particularly when those models lead to substantially different conclusions.

Statistical Models of Army-Relevant Data. The Army has interests beyond those of the general public in several types of data and experiments. The P&S program seeks proposals to develop statistical models and methods for experiment and data types of particular Army interest. Two examples follow, though these are not exhaustive. The first example is in the area of forensic science. The Army is interested in evaluating evidence from criminal investigations involving DoD personnel and from sites that are suspected to harbor adversaries. The P&S research program seeks proposals that will create innovative approaches for source attribution of forensic samples such as drugs, explosives, DNA, or fingerprints; develop methods or protocols for extracting information from mixed DNA samples; develop tools, approaches, and techniques for modeling the statistical assessment of a DNA match with limited information to inform marker and panel selection; develop new quantitative, rather than qualitative, methods for patterned forensic analyses such as firearms, fingerprints, or blood splatters; and develop methods to pre-process, match, and analyze pattern evidence with or without human intervention.

The second example is in the area of wearable monitors. Most data from wearable monitors is analyzed with models in which the data from different people are assumed to be independent of each other. But when many people – e.g. soldiers – perform the same activity at the same time and location in parallel, their data may exhibit dependence. The P&S program seeks proposals to investigate the dependencies, how they can be modeled, and how they can be used to advantage. For example, P&S seeks proposals for distinguishing change points for one person from group-wise change points or for using group-wise data for quicker detection of an individual's change point. P&S also seeks proposals for determining what computing is best carried out locally, on the monitoring unit, as opposed to transmitting all the data to a central computing server. These are just two examples of advancing methods for parallel monitoring data. P&S seeks any proposal that addresses parallel monitoring data. These are just two examples of data types in which the Army has special interest. The P&S program seeks proposals for developing statistical methods to address all types of Army-specific data or experiments. These areas include the Army Modernization Priorities and the DoD Modernization Priority Areas stated in the National Defense Strategy.

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(3) Biomathematics

The introduction of Biomathematics as a separate area of basic research recognizes the importance and specialized nature of quantitative methods, specifically mechanistic modeling, in the biological sciences. Biology involves a large number of entities that interact with each other and their environment in complex ways and at multiple scales.

This complexity makes biomathematics a highly interdisciplinary field that requires unique and highly specialized mathematical competencies to quantify structure in these relationships. In fact, progress in mathematical models of biological systems has traditionally been achieved by making convenient simplifications; major advances in Biomathematics research continue to require removing these assumptions (for example, stationarity, ergodicity and deterministic nature) and finding ways to effectively model the essential complexity. Modeling techniques currently utilized in the field range from agent-based approaches for determining the results of individual behavior, whether those individuals be molecules, zooplankton, or humans, to multi-compartmental modeling in physiology, epidemiology and neurobiology, to network models involved in understanding ecosystem and human social dynamics, as well as encompassing both deterministic and stochastic approaches. Research in control techniques is also valuable for its potential application in militarily important areas such as bio warfare and disease spread. Exciting new opportunities to advance the field are found in high risk attempts to develop modeling techniques in areas of mathematics, such as algebra and topology, not traditionally brought to bear on biological problems, advances in Bayesian statistics, a growing recognition that the diffusion approximation is not necessarily adequate for many systems, and the availability of large amounts of complex biological data.

The ultimate goal of the Biomathematics Program focuses on adapting existing mathematics and creating new mathematical techniques to uncover fundamental relationships in biology, spanning different biological systems as well as multiple spatial and temporal scales. One area of special interest to the program is Neuromathematics, the mechanistic mathematical modeling of neural processes. Recent advances in neuroscience provide important foundations to begin understanding how the brain works. Combined with experimental data, innovative mathematical modeling provides an unparalleled opportunity to gain a revolutionary new understanding of brain physiology, cognition (including sensory processing, attention, decision-making, etc.), and neurological disease. With this new understanding, improved soldier performance, as well as treatments for Post-Traumatic Stress Disorder, Traumatic Brain Injury, and other brain-related disorders suffered by the warfighter will be able to be achieved more effectively, efficiently, and ethically than via experimentation alone.

Thrust areas of the Biomathematics Program are as follows:

Fundamental Laws of Biology. The field of physics has long been “mathematized” so that fundamental principles such as Newton’s Laws are not considered the application of mathematics to physics but physics itself. The field of biology is far behind physics in this respect; a similar process of mathematization is a basic and high-risk goal of the ARO Biomathematics Program. The identification and mathematical formulation of the fundamental principles of biological structure, function, and development applying across systems and scales will not only revolutionize the field of biology but will motivate the creation of new mathematics that will contribute in as-yet-unforeseen ways to biology and the field of mathematics itself.

Multiscale Modeling/Inverse Problems. Biological systems function through diversity, with large scale function emerging from the collective behavior of smaller scale heterogeneous elements. This “forward” problem includes creating mechanistic mathematical models at different biological scales and synchronizing their connections from one level of organization to another, as well as an important sub problem, how to represent the heterogeneity of individual elements and how much heterogeneity to include in the model. For example, the currently increasing ability to generate large volumes of molecular data provides a significant opportunity for biomathematical modelers to develop advanced analytical procedures to elucidate the fundamental principles by which genes, proteins, cells, etc., are integrated and function as systems through the use of innovative mathematical and statistical techniques. The task is complicated by the fact that data collection methods are noisy, many biological mechanisms are not well understood, and, somewhat ironically, large volumes of data tend to obscure meaningful relationships. However, traditionally “pure” mathematical fields such as differential geometry, algebra and topology, integration of Bayesian statistical methods with mathematical methods, and the new field of topological data analysis, among others, show promise in approaching these problems. Solutions to these types of multiscale problems will elucidate the connection, for example, of stem cells to tissue and organ development or of disease processes within the human body to the behavior of epidemics.

The “inverse” problem is just as important as the forward problem. From an understanding of the overall behavior of a system, is it possible to determine the nature of the individual elements? For example, from knowledge of cell signaling, can we go back and retrieve information about the cell? Although inverse problems have been studied for a long time, significant progress has been elusive. This thrust area involves innovations in spatial and/or temporal modeling of multi-level biological elements with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down (data-driven) and bottom-up (model-based) approaches.

Modeling at Intermediate Timescales. Biological processes operate at a variety of timescales; understanding the dynamics of a system at intermediate timescales, as opposed to its long term, asymptotic behavior, is critically important in biology, more so than in many other fields. For example, an epidemic is a necessarily transient phenomenon. In addition, deterministic models are an approximation that often is not good enough to be informative about the system. Yet, intermediate timescales of nonlinear dynamics with stochasticity, both internal and external, are not well understood. This thrust area attempts to fill the gap in the basic understanding of modeling of systems, as well as their control, at intermediate timescales.

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(4) Computational Mathematics

The research strategy of this program is to focus on the following opportunities for crucial discoveries: innovative methodologies for solving currently intractable problems that take advantage of symmetry, conservation, and recurrence, that can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures; novel algorithms that accommodate different mathematical models at different scales, interacting subsystems, and coupling between models and scales; methods that incorporate nonlocality through integral operators with advantageous representations. Research in this area will ultimately lead to the development of new mathematical principles that enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems.

Scientific computation is an essential component of scientific inquiry, complementing theory and experiment, and is also an essential element of engineering in both design and in failure autopsy. Simulations in support of inquiry, design, or autopsy often require expert knowledge in order to select methods that are compatible with the assumptions of the scenario at hand, require considerable skill to properly set up, require considerable time, memory, and storage on large scale parallel/distributed/heterogeneous systems to compute, and require considerable skill and effort to distill useful information from the massive data sets which result. Expert knowledge is also required to quantitatively estimate solution accuracy and to estimate the time and effort required to achieve a desired accuracy. Data has become ubiquitous and is potentially very valuable in increasing solution accuracy and/or decreasing the effort required to solve, but mathematically sound methods for incorporating data into accurate simulations are incomplete. Simulations are not always timely, with results often not being available until after they are needed, for example in calculating failure of New Orleans levees during Katrina and in revising those estimates based on real time surge data. The emphasis in the Computational Mathematics program is on mathematical research directed towards developing capabilities in these and related areas.

For problems that are not time-limited, research areas of interest include but are not limited to the following:

Advances in Numerical Analysis. Novel methodologies are sought for solving currently intractable problems. New ways of taking advantage of symmetry, conservation, and recurrence are of interest, as are new ways of creating sparsity and new computational structures which can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures. Rigorous analysis is sought for each in order to enable error bounds, error distribution, and error control.

Multiscale Methods. Problems of interest to the Army are increasingly characterized by the fact that behavior at microscopic scales has a large influence on performance of systems. To analyze these situations, algorithms are needed to deal with different mathematical models at different scales, interacting subsystems, and coupling between models and scales. The emphasis of this program is on mathematical methods which have some promise of wider application rather than methods limited only to specific application areas.

Fractional Order Methods. As an alternative to high order methods and other less-local operators, fractional operators are another nonlocal operator that have proven to work well in modeling and have the advantage of not enforcing dubious assumptions of smoothness, especially at discontinuities and interfaces. However, the nonlocality of fractional operators also typically introduces a significant increase in computational load. Advances in novel efficient computational methods for these operators are of interest.

Army systems often operate under rapidly-changing unpredictable and adverse conditions. It is desirable for models to be computationally simulated and fast enough to drive decision making, exercise control, and to help avoid disaster. Such simulations need to be created, run, and interpreted in better than real time. Research directed towards making this goal achievable is of interest, such as:

Reduced Order Models. Full scale simulations are often not realizable in real time. In order to investigate the behavior of systems under a variety of possible scenarios, many runs are required. Reduced order models are one way to enable this. Possible methods to create these models include adaptive simplification methods based on singular value decompositions and reduced order numerics. To be useful, all such models should be equipped with reliable estimates of accuracy.

Problem Solving Environments. To enable rapid decision making that is driven by simulation, it is necessary to set up simulations very quickly and obtain results in an understandable format. Matlab is one current tool for such a problem solving environment. What are other approaches?

Embedded Simulation. As algorithms become more efficient and computational devices shrink, it will become increasingly possible to use real-time simulation to drive control systems. New methods which address this goal are welcome, especially those which permit user- controlled and/or adaptively-controlled tradeoffs between speed and accuracy.

Decision Making. One valid criticism of numerical simulation is that it takes so long to set up, run, and post-process the results that they cannot be used in a timely manner to guide decision making. Mathematical ideas that help address this problem are of interest.

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iii. Network Science

The objective of the Network Sciences Division is to discover mathematical principles to describe ever present networks in all walks of life (e.g., organic, social, electronic) and, in particular, the emergent properties of networks. Study of Network Science is necessarily multi-disciplinary drawing on tools and techniques from statistical mechanics, information theory, computer science, control theory and social sciences to studies interactions at large scale, be they in swarms of insects or ant colonies, human societies, or networked autonomous systems. The basic principles discovered should, in turn, lead to creation of algorithms and autonomous systems that can be used to reason across data generated from disparate sources, including, sensor networks, wireless networks, and adversarial human networks. Research in this Division has applications to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals engendered by principles such as the Net-Centric Warfare and Third Offset strategy.

Research in the Network Science Division, while primarily driven by discovery of foundational principles, will, however, be cognizant of and contribute to providing crucial underpinning support to ARL's Network & Information Sciences Competency. In particular, the following goals within ARL's Network & Information Sciences Competency are explicitly addressed including: (i) assessment and control of behavior goal by creating new methods in design and controllability of composite and multi-genre networks; (ii) social effects and human-machine interaction through the exploration of social and cognitive networks, and generation of intelligent actions in a mix of information agents and humans; (iii) unconventional communication networks and adaptive by making information available at the tactical edge while taking limited bandwidth and human-information interaction modalities into account, and (iv) taming flash-flood of information available at the tactical edge.

The Network Science Division hosts four main programs in Wireless and Hybrid Communication Networks, Social and Cognitive Networks, Intelligent Information Networks, Multi-Agent Network Control, and an international research program in Network Science and Intelligent Systems. The boundary between these programs is fluid and, thus, a research topic might fall in more than one program area. Furthermore, there are shared interests between the Social Sciences program in Physical Sciences Directorate and Social and Cognitive Networks (SCN) program in Network Science, with SCN paying special attention to the human dimension from a network science perspective, including study of connections between interdependent people (such as teams), between social systems and cognitive processing (such as collective learning and decision making), and between humans and machines, using tools and techniques from computer science to further the study of social and cognitive processes of humans embedded in large social, interconnected systems. It is perhaps worth emphasizing that research which elucidates and defines the common underpinning science cutting across different types of networks is particularly of interest to Network Science Division.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in network science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Communications and Networks

This program is concerned with the investigation and advancing of network science applied to communication networks, in particular in wireless and tactical environments, with focus on Department of Defense and Army unique problems. These include, but not limited to, infrastructure-less wireless networks operating in congested and contested spectrum. Also of interest is the analysis of mutual interaction among the communications, social and information networks.

Wireless Network Theory. Research is required in the broad area of wireless network science including fundamental limits, performance characterization, novel architectures, and high fidelity simulation of multi-hop wireless networks with mobility, node loss, natural and man-made impairments and unpredictable, bursty traffic. Of particular importance is the extension of these findings in millimeter wave networks where spectrum is abundant, but connections are fragile and distances are short. Novel analytical tools and simulation techniques may be necessary to allow for the modeling of very large networking scenarios without losing the fidelity at the physical layer, which is critical in millimeter wave networks.

Emerging communications network paradigms of Software Defined Networking (SDN) and Network Function Virtualization (NFV) are also of interest as applied to wireless and hybrid networks. Concepts from SDN/NVF could be adapted for wireless ad hoc networks, using innovative methods. Complete centralization may not be desirable, but policy control and hierarchical control of semi-autonomous systems could be useful. Exploitation of SDN control architecture to tailor virtualized network resources according to the needs and objectives of the users is desired. Also, exposure of signaling traffic in wireless SDN creates significant security challenges which need to be resolved.

Mobile Ad Hoc and Sensor Networks. Networks serving Army needs operate in highly dynamic environments with limited or no infrastructure support. Available spectrum may be highly congested and contested, and mobile nodes may only have access to noisy local information with limited awareness of remote nodes in the network. Novel networking approaches may be needed to account for the lack of full network state information and reduce the penalty incurred due to coordination while sustaining acceptable performance.

Adaptive and specialized machine learning techniques are needed for dynamic allocation of network resources based on operation needs, traffic characteristics, mobility, natural and man-made spectrum interference conditions, and security considerations. Techniques to discover and capitalize on communication and networking opportunities. Networking and sensing architectures for cognitive mobile ad hoc networks needs to be developed with qualitative and quantitative performance measures, and the impacts of mobility, fading, and multi-user interference needs to be investigated. Concepts and constructs observed in networks encountered in nature could inspire adaptation strategies for ad hoc wireless networks.

Networking in combat operations may need to cope with the presence adversarial actions of various types, including strategically inserted spectral impediments. New signal processing, information theory, game theory and network science methodologies are needed to provide reliable and efficient communications in the presence of various adversarial actions. The analysis and characterization of fundamental tradeoffs among conflicting objectives such as Low Probability of Detection (LPD) vs. rate of communications vs. operating in a limited frequency spectrum are needed, along with novel techniques to achieve optimally located areas in the trade-off boundaries.

Providing energy efficient sensor networking under possibly hostile operating conditions presents considerable challenges. Such networks involve short packets and very large number of users, for which standard network access methods are known to be neither spectrum, nor energy efficient. Investigation of fundamental limits in network access methods which pertain to short packets, many users and hostile environments is desired, along with the discovery of protocols which could approximate these bounds.

Novel and Revolutionary Methods in Networking. The synergy among social networking and communication networking, particularly in a tactical mobile ad-hoc scenario, is a research area that could advance the design of new communication approaches. There are many social networking aspects that are common to mobile ad-hoc networking needs such as distributed decision making, robustness, cooperation, self-organization, cluster formation, search and exploration, to name a few. Social Networking Analysis concepts have been recently used in routing and storing of information for tactical wireless networks, with some encouraging results.

Distributed authentication methods, such as block-chain could be useful in tactical environments, but they may require excessive computation and storage burden. Rethinking of distributed authentication methods to fit tactical environments where links may be unreliable, energy and storage is limited is desired.

Among novel and revolutionary methods in networking, exploration of quantum information processing, teleportation and networked quantum information theory is of interest.

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(2) Social and Cognitive Networks

The goal of the Social and Cognitive Networks program is to understand human behaviors and cognitive processes leading to collective level phenomena particularly relevant in military settings with an emphasis on high performance teams and computational social science. Social networks are the underlying structure of interaction and exchanges between humans within both strategically designed and emergent or self-organized systems. Social networks allow for collective actions in which groups of people can communicate, collaborate, organize, mobilize, attack, and defend. The changing nature of DoD's missions greatly increase the need for models that capture the cognitive, organizational, and cultural factors that drive activities of co-present, virtual, or distributed groups, teams, and populations. Better understanding the human dimension of complexity will provide critical insights about emerging phenomena, social diffusion and propagation, thresholds, and tipping points.

The Social and Cognitive Networks program supports projects that contribute substantive knowledge to theories about human behavior and interaction and make methodological advancements in modeling and analyzing social network structures. The U.S. Army is particularly interested in research that uses defense-relevant empirical data to feed into computational and mathematical models of human interaction. As such, this program funds projects successful in blending theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. Advances in this program are expected to lead to development of measures, theories, and models that capture behavioral and cognitive processes leading to emergent phenomena in teams, organizations, and populations.

Human Behavior and Interaction. This program supports research from disciplines such as communication, health and behavioral science, I/O and social psychology, library and information science, management science, and sociology that use a social networks lens to focus on the ways people think and interact whereby creating higher-order systems. Topics of interest include social influence, leadership, trust, team science, cooperation and competition, and crisis management. Such social influence and opinion dynamics research could focus on the formation and dissolution of civic-minded and violent ideological networks, mobilization of benign to hostile political movements, propagation of and enduring changes in attitudes leading to populations reaching consensus or contested states, and network-based interventions. Furthermore, topics of particular interest include social effects of human-machine teaming; multi-team systems and multilevel (nested) systems; and health topics related to education, healthcare behaviors, disease propagation, and wellness from a social networks perspective.

Information and Knowledge Management. This program supports social network centric research to study the ways people learn individually and collectively and how they utilize that information for decision making and goal attainment. Examples of relevant topics include transactive memories, public goods, collective action, information sharing, information fidelity, diffusion and propagation dynamics, and collective decision-making. Diffusion dynamics research will develop mechanistic understanding of opinion and behavior change associated with influence, contagion, and other social propagation processes. Collective decision-making research will contribute fundamental theories and models to predict, evaluate and simulate how teams organize, exchange information, build knowledge, influence, adapt, learn, and build consensus using cooperative strategies and emergent capabilities.

Social Network Analysis. In addition to the topical areas identified above, this program supports methodological advancements for social network analysis. Methodological research in this program will focus on important advances in exponential random graph models (ERGMs or *p**), object oriented agent-based models, computational models, and dynamic simulations that resolve network modeling issues. Such research will focus on scalability of networks, hierarchical or multilevel (nested) systems, longitudinal networks, social influence models, network resilience, techniques to deal with missing, incomplete, or inaccurate network data, and techniques to deal with visualizing multilevel multimodal networks. Scalability and dimensionality research will identify overarching mechanisms that span scales and dimensions of human systems that will parameterize, model, and predict both small group and big data network models. Data accuracy research focuses on investigating effects of measurement error on metrics and inferences due to incomplete (missing or inaccurate) network data. These projects could include research examining small group dynamics within big data sets; multi-level models that account for nested cognitive, social, cultural, physical dimensions of systems; or link and subgroup estimation algorithms to deal with incomplete data and clandestine activities.

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(3) Information Assurance

From the Army perspective, Information Assurance must provide authentic, accurate, secure, reliable, timely information to warfighters in order to achieve information dominance, regardless of threat conditions. Computing and information processes may be carried out over distributed and heterogeneous systems, which may include mobile computing and communications systems, and high performance information process systems that are inter-connected through both tactical and strategic communication systems.

Robust and Trusted Wireless Communication. Research is needed in the areas of theory, protocols, and techniques that will assure delivery of trustworthy data to support battlefield missions. Reconfigurable, survivable, and self-healing systems allow a combat unit to dynamically establish and maintain its command and communication capability under diversified and extreme battlefield situations. The Army requires a fully mobile, fully-communicating, agile, and situation-aware force that operates in a highly dynamic, network centric environment. This force consists of a heterogeneous mixture of individual soldiers, ground vehicles, airborne platforms, unmanned aerial vehicles (UAVs), robotics, and unattended sensor networks such as battlefield IoTs that operate in a complex wireless environment. Information theory has played a foundational role in the study of security. Across a wide range of application domains and security objectives, information theory leads to insight to the underlying tradeoffs between security and performance. The Army seeks novel ideas in fundamental research areas such as information-theoretic security and the science of security that will provide direct guidance in the design of secure tactical wireless systems. In particular, topics of interest include new paradigms for physical layer security (ranging from confidentiality to authentication to trustworthiness in physical layer communications), the fundamental bounds in key management in distributed systems, the exploitation of key establishment and distribution protocols, and trusted information delivery and dissemination in mobile environments. The corresponding constructions that would arise from such an investigation represents a significant avenue for improving future wireless communication as well as the corresponding secrecy capacity limits that could serve as valuable guidelines in developing future systems with confidential and authenticated communications. New computing and communication protocols and techniques are needed to assure critical information processing and delivery even when such systems are under severe resource constraints or under persistent attacks.

Models and Metrics for Next Generation Survivable Systems. The field of information assurance needs a foundational science to guide the design of systems and to quantitatively measure safety and the level of assurance of complex systems that the Soldier depends upon today. Assurance principles and metrics are needed to help define, develop, and evaluate future robust and resilient systems and network architectures that would survive sophisticated attacks and intrusions with measurable confidence. The program seeks the capability to measure a complex system and to produce a scalar value that can determine the trustworthiness of that system. In addition, human users need to be in the loop for system assurance analysis. Developing human centric security-usability metrics, computational models for usable security in stressful situations, and adaptive security protocols according to perceived threats are some of the research areas of interest for improving warfighter performance while maintaining sufficient security requirements. One new challenging area of research that offers great promise in stronger system robustness is the modeling of adversaries and defender interactions, since ultimately systems need to defend effectively against their attacks. A deeper understanding and more accurate modeling of adversarial behaviors will improve future system development.

Cyber Deception. Cyber deception is a proactive technique to manipulate the mental state and decision process of the adversary so that we can degrade and mitigate their attack effectiveness. Unique aspects of cyber deception may offer more opportunities but add more complexity to model and analyze: 1) Cyber artifacts (both genuine and fake) can be created easily and are not bounded by the laws of physical space. The velocity of cyber situation change could be very high; 2) while deceptions are normally played out between a defender and an attacker, users could be directly or indirectly entangled in the game due to the nature of shared infrastructure. Usability issues or negative impact to the mission need to be considered; 3) Social and cultural aspects are important elements in the cyber deception game. Key scientific understanding is still lacking in 1) Establishing effective mental models for understanding and tracking the adversaries' intent, capability, and decision process, and 2) deception information formulation and communication techniques, which requires new thinking in order to provide a quantifiable measure on how a given deception approach will drive metal state change. Recent honeypots/decoy experiences gave initial insights on how to engage adversaries through fake cyber artifacts, but a clear understanding of the dynamics (especially mental interactions) between attackers and defenders is missing. A better learned adversarial model will be critical to the success of cyber deception. In addition, advanced honeypot like schemes are desired to engage adversaries in order to gain understanding of adversaries so that effective deception schemes can be crafted.

Principles of Moving Target Defense. Current cyber defenses are often static and governed by lengthy processes, while adversaries can plan their attacks carefully over time and launch the attacks at cyber speeds at times of their choosing. The program seeks a new class of defensive strategies to present adversaries with a moving target where the attack surface of a system keeps changing. Although such an idea of a "moving target" is a powerful paradigm for building systems robust to security threats, many fundamental aspects associated with such a strategy need to be further investigated and understood. For example, such a "moving target" system may operate under many different contexts, ranging from the use of frequency hopping in spread spectrum to software diversification. It is critical to establish new theories and models that can provide trade-off analysis between system robustness against attacks vs. performance/usability, and quantify the risks associated with system adaptation under an adversarial setting. Ultimately the understandings and analytical models obtained will establish an important foundation for creating robust tactical systems capable of maximizing the difficulties for the adversaries to attack while minimizing the impact to system performance and usability.

Trusted Learning for Cyber Autonomy. Given a massive amount of data coupled with strong computation power, machine learning (ML) algorithms such as deep neural networks have shown initial success in many applications. However, without considering an adversarial setting, studies have shown fatal vulnerabilities in current AI systems where a small adversarial perturbation can easily fool current AI into making wrong decision. The main contributing factors to AI vulnerability are: 1) the black box data driven approach provides no guarantee of either correctness nor security assurance; 2) current learning regime is extremely brittle since it assume that both training testing data are from the same stationary i.i.d. distributions commonly violated in real world, especially under an adversarial setting; 3) given an ultra-high dimensional data space, blind data spots do exist from training and can be easily exploited by adversaries. Given the serious adversarial risks to ML based systems, it is critical to carefully re-examine and rethink the fundamental aspects of ML that leads to its brittleness. It is critical to study and establish adversarial models which is the most critical first step in defense so that both correctness and robustness in learning and decision making for cyber defense can then be quantified. New scientific understandings are sought in terms of attack resilient learning, decision making and cyber autonomy, both at the data driven layer and the knowledge layer so that cyber defense relying on learning and adaptation will be more robust and resilient against adversarial manipulation and exploits.

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(4) Multi-Agent Network Control

The objective of the Multi-Agent Network Control program is to establish the physical, mathematical and information processing foundations for the control of complex dynamic networks with possibly multiple controllers. The research program is concerned with developing novel mathematical abstractions and methods for the modeling and control of the collective behavior of large scale networks of heterogeneous multi-agent systems. Autonomy is central to program efforts as anticipated dynamics of the future battle space will require a greatly increased level of autonomy to enable the necessary mobility, sensor coverage, information flow, and responsiveness to support the military goals of information superiority, dominant maneuver, and precision engagement.

Distributed Control of Networked Systems. Distributed control techniques have played a major role in the study of networked systems. For example, they have been successfully used in robotics for replicating self-organized behaviors found in nature (e.g. bird flocking, fish schooling, and synchronization) and in developing applications such as formation control, rendezvous, robot coordination, and distributed estimation. In many dynamic systems, consensus based solutions may not be applicable, due to time varying and abrupt transitions of the states, hard to quantify uncertainties and unknown objectives of the agents. More sophisticated distributed control methods that go beyond consensus formulations are needed. Analysis of interactions between information and control is a fundamental research topic with implications in distributed systems design. Methods for computing bounds and derivation of optimal or near optimal solutions under incomplete and local information for agents, as well as design techniques that quantify trade-offs between information delivery costs and system optimality are of interest. Analysis of distributed non-linear systems where linearization is not applicable is also sought, using innovative techniques such as geometry, graph theory, topological analysis and possibly others. Also of interest are modeling and analyses of interacting and co-evolving multi-genre networks that have their own focuses and functions, but nevertheless interact with each other in the realm of distributed control.

Adaptive Control and Reinforcement Learning. Control of uncertain systems in conjunction with methods to reduce uncertainties is part of mainstream control systems research, one example being Reinforcement Learning (RL). Stochastic Dynamic Programming approach has led to powerful formulations in RL, with impressive results in many applications. This success is partly shadowed by issues such as computational complexity, very long convergence times, and lack of sufficient training data, especially in Army related applications. Hybrid approaches that properly incorporate prior or learned models of the systems to be controlled into the RL formulation are encouraged. Research to address fundamental issues in RL such as computational complexity, convergence times and training with sparse data are sought. Also, novel approaches to RL which may extend, modify or replace state space based Dynamic Programming paradigms are desired. Extensions of RL techniques to networked systems featuring multiple controllers with applications to autonomy and coordination are sought. Innovative research focused on system identification techniques to reduce uncertainty and facilitate optimal or near-optimal control is also within the scope of this program.

Novel Application Areas in Control Theory: Sophisticated tools and methodology resulting from research conducted in control could conceivably provide new insights and their extensions and adaptations could be helpful towards the solutions to some important and challenging problems. Such problems include, but are not limited to, control and stability of Quantum Qubits and delineation of control functions occurring in the brain. Computational capabilities enabled by computers built using Quits are expected to far surpass classical computing facilities. However, control and stability of clusters of qubits remains a fundamental problem in quantum computing. Adaptation of control theoretical tools and approaches into precise control of qubit spins and into extending the stability of coherence times of interacting qubits could provide new research opportunities in the control of systems with interacting elements. Cognitive functions in the brain are controlled by interactions among neural circuits, but fundamental principles describing these interactions are not currently well understood. Modeling and analysis of these phenomena could provide novel research opportunities in the control of networked systems. Similarly, study of biological systems unveil control architectures that are not encountered in industrial control systems. Understanding the effectiveness of such natural control systems and their potential adaptation to the control of man-made applications could also be an area of fertile research.

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(5) Network Science and Intelligent Systems (International Program)

As one of the ARO International Programs, the Network Science and Intelligent Systems Program is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward looking and promising research in network science.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

2. INTERNATIONAL RESEARCH INTERESTS

The U.S. Army Research Office has international research programs which are focused in specific research areas supporting the 10 scientific divisions. These research areas and information provided in the following are opportunities for foreign organizations and foreign public entities.

a. Energy Transport and Storage

As one of the ARO International Programs the Energy Transport and Storage Program is focused on supporting research at universities outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which energy storage and power generation technologies depend. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

This program targets insightful and high-risk, fundamental research which addresses the core underlying limitations of energy transport/storage. Central to the mission of this program is the exploration of how materials and cell design can be tailored to enable targeted electrochemical reactions—while eliminating side reactions, hazards and other impediments, thereby surmounting hurdles and exploiting opportunities in chemical energy storage.

Energy Transport. This thrust supports research aimed at evaluation protocols for energy-relevant materials and the scrutiny of new solid ion conductors and liquid/slurry active materials. There is a tendency to focus upon the most favorable aspects of energy-relevant chemistries and materials, but such reports often either fail to identify or neglect the key limiting characteristics which researchers in general and the Army in particular require to overcome the constraints which restrict breakthroughs in a given energy technology. Projects which actively seek to obtain a global understanding of the underlying principles regarding how chemicals/materials impact the stability and performance of energy storage technologies are of Army interest. Advances in solid electrolytes hold the promise of revolutionizing energy storage technologies, but numerous factors such as limited ionic conductivity, poor ion selectivity, high reactivity, composition changes during processing or difficult processing methods, high contact resistance, unfavorable mechanical properties, defect propagation during cycling due to mechanical deformation, cost barriers, etc. remain major obstructions to the integration of solid electrolytes/separators into devices. Innovative approaches to propel these critical cell components forward are sought. The identification of promising, new liquid (or slurry) active materials (i.e., anolytes or catholytes) may potentially enable new cell designs which greatly simplify battery production, scalability and the tunable modularity of cells, thus enabling their assimilation into diverse Army-relevant energy storage applications. Other innovative project themes are also welcome.

Thermal Energy Storage. This thrust's focus is on thermal energy storage phase change materials (PCMs). PCMs permit both passive and active heating/cooling that can significantly reduce or eliminate the necessity of conventional heating and cooling methods (for buildings, refrigeration, electronics, etc.). Many PCM applications, however, are restricted due to their high cost, low thermal conductivity, change in density, limited stability of thermal properties and tendency to subcool. The discovery and characterization of new PCMs (e.g., based upon solvates, eutectics, etc.) may overcome these challenges thereby enabling a path forward for their widespread implementation.

TPOC: Dr. Wesley Henderson, wesley.a.henderson4.civ@mail.mil, +81-46-407-9310 (Tokyo, Japan)

b. Synthetic Biology

As one of the ARO International Programs the Synthetic Biology Program is focused on supporting research at universities outside of the U.S., building international partnerships and laying the foundational work on which applications of synthetic biology will depend. Emphasis is on using synthetic biology techniques to understand basic biology and to design biological systems and processes with high reliability, scalability, and predictability. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

A major program thrust is investigation of the ways in which biological systems use and control evolutionary processes to become robust, complex, and adaptive. Investigations of interest include mutational hot spots, genetic rearrangement, horizontal gene flow, hyper stable DNA regions, recurrent editing, and maintenance through generations of "unused" adaptations, for example adaptations that allow resistance to dehydration maintained for generations in the absence of selective pressure. These naturally occurring processes may be combined with techniques that do not occur in nature, such as gene shuffling and directed editing, to create organisms that are both engineered and adapted. Combined with a systems biology approach, principles of encoding complexity and adaptivity can be derived. Sophisticated selective techniques are also sought, to drive evolutionary processes to desired ends and to create organisms with desired characteristics.

A second research thrust is the development of robust, predictable systems. Emphasis is not on what such a system does so much as how it can be created, maintained, and activated, to include consideration of the time course of reactions, energetics, methods of preservation and storage, methods of activation, stability, and reliability.

The third thrust of the program is on the creation and maintenance of hybrid prokaryotic-eukaryotic symbiotic systems. Such systems can potentially combine the relative ease of engineering of prokaryotes with the robustness and processing capability of eukaryotes. Areas of interest include the reliable formation of stable intracellular prokaryotic forms, release and reformation of extracellular prokaryotic forms, transport of prokaryotic products into eukaryotic cytoplasm, membranes, and extracellular space, and eukaryotic processing of prokaryotic products. Studies of the innate immune system of both plants and animals are also of interest, as well as intracellular immune processes.

TPOC: Dr. Valerie Martindale, valerie.e.martindale.civ@mail.mil, +81-46-407-9309 (Tokyo, Japan)

c. Human Dimension

As one of the ARO International Programs and part of the ARO Life Sciences Division portfolio, the Human Dimension Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of identifying and modeling the co-evolutionary multiscale dynamics of human neural, cognitive, physical and social systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Human Dimension Program supports multidisciplinary basic research in areas that include neural and cognitive sciences, behavioral and social sciences and human factors and neural engineering with an emphasis on modeling, predicting and enhancing human perceptual, cognitive, affective, physical, and social performance in individuals, groups and societies. An overarching goal of the program is to provide foundational knowledge of neural, biophysiological and cognitive-based mechanisms underlying individual, group and societal cognition and performance across multiple time scales. In the long term, research in this area may enable new training tools to predict and optimize cognitive/physical performance and team intelligence, interfaces enabling humans to more efficiently control machines and psychophysiologically-based predictive models of complex individual – societal dynamics. Basic research opportunities are sought in two primary research thrusts within this program: (i) Cognitive-Physical Interactions and (ii) Cognitive-Social Interactions.

Cognitive-Physical Interactions. The Cognitive-Physical Interactions thrust seeks to support high-risk seed projects that use multimodal approaches to uncover dynamic and multiscale interactions of neural-cognitive and physiological systems. The goal of this thrust area is to advance the experimental and analytical tools available to develop comprehensive understanding of the impact of group and individual state-trait variability on human performance, human-systems interfaces and team intelligence. Research topics are supported in diverse areas that can include the neurobiological mechanisms of expert skill learning, closed-loop brain-computer interfaces and novel mind-body interfaces such as the microbiome-gut-brain axis.

Cognitive-Social Interactions. The Cognitive-Social Interactions thrust seeks to develop new theories to understand the dynamic interrelationships between individual/group cognition, decision-making and the role that these influences play on interactions with large and small social systems. Multidisciplinary seed projects are supported that seek to advance the necessary analytical and experimental tools required to describe the underlying mechanistic interactions as they co-evolve in time and space. Research topics are supported in diverse areas that may include modeling the impact of mindfulness on state transitions of human cognitive, physical and social systems and describing the longitudinal neural, cognitive and social mechanisms mediating development of leadership, expertise and intelligent teams.

TPOC: Dr. Frederick Gregory, frederick.d.gregory5.civ@mail.mil, +44 (0)1895-626517 (London, UK)

d. Quantum Scale Materials

As one of the ARO International Programs the Quantum Scale Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in quantum scale materials. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Specific research topics of interest include, but are not limited to: topological states of matter and photons, matter and photons that can support anyon quasiparticles, quantum phase transitions, non-equilibrium quantum dynamics, novel materials for quantum information processing, quantum metrology with atoms, ions and photons, quantum networks, and novel quantum information effects, such as effect of free will (measurement independence) on quantum algorithms, such as teleportation, quantum communication and quantum computing.

Additionally, over time new areas of research in fundamental physics surface that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases.

TPOC: Dr. Thomas B. Bahder, thomas.b.bahder.civ@mail.mil, +81-46-407-9308 (Tokyo, Japan); (984) 209-0096 (U.S. cell)

e. Innovations in Materials

As one of the ARO International Programs the Innovations in Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of accelerating new discoveries in materials science. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Innovations in Materials program seeks to determine unique strategies and designs for optimizing materials with uncharacteristic or unexpected properties, architectures, and compositions. Research is focused on, but not limited to, areas such as: reconfigurable materials, predictive design of materials, multi-component materials incorporating hierarchical constructs, materials compositions and architectures for unprecedented property development, functional integration of materials, analytical techniques for interrogating multi-dimensional evolution of structures, properties and failure, and defect science and engineering.

Over time, new areas of research in fundamental materials science can develop that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases as well.

TPOC: Dr. Pani Varanasi, chakrapani.v.varanasi.civ@mail.mil, (919) 549-4325

f. Network Science and Intelligent Systems

As one of the ARO International Programs the Network Science and Intelligent Systems program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in network science and intelligent systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Wireless Communications and Information Networks. Networks serving Army needs must operate in highly dynamic environments with limited infrastructure support. Networks will be disconnected, intermittent, and limited (DIL) environment, with limited state information and dynamic network connectivity and intermittent link connectivity as well as dynamic traffic load with various QoS constraints and priorities. Metrics, fundamental limits, and performance need to be characterized for tactical networks as well as new theory that will lead to reliable and efficient communications that meets QoS constraints. New algorithms and protocols that are more robust in the presence of various adversarial attacks are required.

One specific area of interest is SDN that can operate within tactical DIL networks. Standard SDN are centralized utilizing a reliable control plane, which are not available in this environment. Research is needed to investigate if SDN can be used in this environment and how architectures and control algorithms need to be modified to meet QoS requirements.

Social Network Analysis and Visualization. Mathematical models for dynamics of large social networks are of interest. Modeling of dynamics of the social network are of interest to include both (and possibly co-evolving) structure and content (e.g., opinion dynamics). Hierarchical, multi-level, and composite network models are of interest to model interactions between networks. Scalability issues should be investigated to understand when they are applicable and models should be vetted against established sociological concepts and, if possible, using experimental data. Multi-scale visualization of social network data is important for presenting results of analysis to users and assisting in manual analysis. Missing, incomplete, and inaccurate data are issues that should be considered in network analysis techniques.

Dynamics of Interdependent and Multilayer Networks. In the emerging field of networks science, the importance of research into interdependent and multilayer networks, such as communications, social, and infrastructure networks, is becoming evident. The mathematics to understanding how to model, predict, and control such multi-layer and interdependent networks is an important research area.

Intelligent Systems. This part of the BAA invites proposals in the area of Network

Inference, Data Mining, and Algorithmic Game Theory that supports aspects of Network Science, including understanding large groups, especially adversarial non-state actors. Work that advances Network Science by bringing new techniques from Game Theory, Machine Learning, Graph Algorithms, Reasoning under uncertainty, are welcome.

TPOC: Dr. Derya Cansever, derya.h.cansever.civ@mail.mil, (919) 549-4330

3. ARO SPECIAL PROGRAMS

a. Short-Term Innovative Research (STIR) Program

The objectives of the STIR program are to support rapid, short-term investigations to assess the merit of innovative new concepts in basic research. STIR program awards provide an excellent opportunity to showcase new concepts and explore new areas in basic research. Historically STIR program awards have helped shape new directions in research for the Army.

i. Eligibility. Proposals are sought from institutions of higher education, nonprofit organizations, state and local governments, foreign organizations, foreign public entities, and for-profit organizations (i.e. large and small businesses). Prospective applicants of a STIR proposal are encouraged to contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA, to ascertain the extent of interest in the specific research project.

ii. Research Sought. Proposals in the amount of $60,000 or less are sought for research in the areas identified earlier in the research areas of this BAA.

iii. Proposal Preparation.

(1) Eligible applicants should submit proposals that are no more than twenty (20) pages in length, inclusive of the budget, transmittal letter, and attachments. No brochures or explanatory material should be submitted with the proposal.

(2) Proposed research efforts must be "stand alone" and not predicated on the use of any facilities other than those under the direct control of the applicant. Research must be completed within nine (9) months of award of the agreement.

(3) The research proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA. Limited rights in technical data and restricted rights in computer software should be identified as an attachment to the proposal. Otherwise, it will be concluded that the proposal does not contain any such limitations or restrictions

(4) No capital equipment may be purchased under a STIR Program award. Travel costs must not exceed $500. Report preparation costs must not exceed $100. Fee is not permitted under STIR Program awards. Due to the relatively small dollar amount and short-term nature of these awards, applicants are encouraged to maximize the benefit derived from this funding by

prioritizing labor and employing other cost-saving measures in support of the STIR program effort. In particular, applicants are strongly encouraged to contribute as a cost-share or significantly reduce the indirect costs associated with proposed efforts.

(5) The principal investigator(s) (PI) should disclose and explain the relevance of the proposal to the research interests identified earlier in the research areas of this BAA.

(6) A brief, final technical report is required. Please note that your award document will reference Form 18, "Reporting Instructions," as found at http://www.arl.army.mil/www/default.cfm?page=29 You shall use these reporting instructions for format instructions only; the due date for receipt of a final technical report is thirty (30) days from completion of the award.

b. Young Investigator Program (YIP)

YIP awards are one of the most prestigious honors bestowed by the Army on outstanding scientists beginning their independent careers. The objective of the YIP is to attract outstanding young university faculty members to pursue fundamental research in areas relevant to the Army, to support their research in these areas, and to encourage their teaching and research careers. Young investigators meeting eligibility requirements may submit a YIP proposal. Outstanding YIP projects may be considered for a Presidential Early Career Award for Scientists and Engineers (PECASE). For FY20 only, this program will be supplemented by additional funding provided by the Defense Established Program to Stimulate Competitive Research (DEPSCoR). Three additional awards may be made to principal investigators in DEPSCoR-eligible states as defined in 10 U.S.C. 2358, as amended by Pub. L. 115-91, div A, title II, sec. 219. Potential awards will be limited to Institution of Higher Education (IHE) in States/Territories that are eligible under the DEPSCoR program authority. Tenured or tenure-track faculty members with appointments at IHE, in the following States/Territories, are eligible to apply for DEPSCoR opportunities: Alabama, Alaska, Arizona, Arkansas, Connecticut, Delaware, District of Columbia, Guam, Hawaii, Idaho, Indiana, Iowa, Kansas, Kentucky, Louisiana, Maine, Minnesota, Mississippi, Missouri, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Oregon, Puerto Rico, Rhode Island, South Carolina, South Dakota, Tennessee, U.S. Virgin Islands, Vermont, West Virginia, Wisconsin, and Wyoming.

i. Eligibility. This program is open to U.S. citizens, U.S. Nationals, and Permanent Resident Aliens holding tenure-track positions at U.S. institutions of higher education, who have held their graduate degrees (Ph.D. or equivalent) for fewer than five years at the time of application. Faculty at an institution of higher education which does not designate any faculty appointments as "tenure track" are eligible if that fact is so indicated in the proposal, and the supporting letter from the institute states that the faculty member submitting the proposal will be considered for a permanent appointment.

ii. Research Sought. Proposals are encouraged for research in areas described earlier in the research areas of this BAA. Proposals may be submitted at any time. As is the case for all other research programs, discussions with the cognizant TPOC/ Program Manager identified earlier in the research areas of this BAA is strongly recommended before submission of a formal proposal. An award in each topic area is not guaranteed. YIP awards will not exceed $120,000 per year for three years.

iii. Proposal Preparation.

(1) An individual applying for a YIP award must submit a proposal and a supporting letter, both through official channels in the institution of higher education where the individual is employed. Any resulting award will be made to the institution, not to the investigator. The proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

(2) The supporting letter must be from the individual's Department Chairperson, Dean, or other official who speaks for the institution of higher education, and should address support for, and commitment to, the applicant. Strong university support for the applicant is essential. This support can include the applicant's nine-month academic salary, release time from administrative responsibilities, the purchase of equipment, support for the applicant's graduate students, waiver of indirect costs, departmental cost sharing, start-up funding, and so on. It must be clear that the institution of higher education views the individual as a truly outstanding, faculty member, and is making a long-term commitment to the proposal and the research.

iv. Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and Section II.E.1.b of this BAA. YIP proposals will be selected for award on a competitive basis after a peer scientific review.

v. Continued Support. Support under the YIP is limited to three years. Upon completion of the YIP award, a young investigator, through their institution, may apply and be considered for continued support in the research areas of this BAA.

c. Presidential Early Career Award for Scientists and Engineers (PECASE)

i. An individual may not directly apply for a PECASE award. Instead, once a year, ARO technical program managers will nominate PECASE candidates from among all ARO YIP and other proposals and whitepapers (if any) received. A technical program manager will make the PECASE nomination based on strong endorsement of the proposal by the external scientific reviewers and on the potential shown by the individual to contribute to science and to the mission of the Army.

ii. Following nomination of a PECASE candidate, a supplemental PECASE proposal will be requested in which the candidate will indicate how PECASE funding would augment the YIP award. PECASE awards are not to exceed $200,000 per year for five years. The following supporting information at minimum is required in the PECASE proposal:

(1) Letters (non-federal government) of recommendation;
(2) Detailed scientific biographical information including a description of the candidate's leadership in the scientific community;
(3) Description of the proposed candidate's publications (such as refereed journals, peer-reviewed conference papers, and books or book chapters; however, this is not an inclusive list);
(4) Description of the candidate's presentations (such as invited talks and plenary presentations; however, this is not an inclusive list);
(5) Summary of the candidate's past research accomplishments;
(6) Summary of the candidate's community outreach efforts; and
(7) Letters of commitment from institution(s) of higher education.

iii. Complete PECASE proposal packages will be evaluated by scientific reviewers. The proposals which demonstrate the greatest potential to contribute to science and to the mission of the Army will be rank ordered by an Army PECASE Evaluation Committee. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.d of this BAA.

iv. Continued Support. Support under PECASE is limited to five years from date of award. Upon completion of the PECASE award, an individual, through their institution of higher education, may apply and be considered for continued support in the areas identified earlier in the research areas of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

d. Research Instrumentation (RI) Program

RI is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense. Of the funds available to support ARO mission research described in this BAA, funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities.

i. Eligibility and Areas of Interest. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of an instrumentation proposal.

ii. Content of Request for Instrumentation. The request for instrumentation shall include:

(1) A concise abstract (approximately 300 words but not to exceed 4,000 characters) that describes the instrumentation requested and the research to be supported by that instrumentation.

(2) A budget that addresses the instrumentation to be purchased, cost per item, and total cost. Indicate the proposed source of the instrumentation and the name and telephone number of a contact at that source. The budget should indicate the amount of funds to be contributed by other sources toward the purchase of the instrumentation.

(3) A description of how the proposed instrumentation will: (i) establish new research capabilities, (ii) contribute to research currently proposed to DoD, or (iii) enhance the quality of research currently being funded by ARO.

(4) A description of how the proposed instrumentation will interface with or upgrade other research facilities and instrumentation now available.

(5) A description of the amounts and sources of ongoing or proposed support for the research to be supported by the instrumentation.

Note: Costs associated with equipment/facility modifications are generally considered unallowable and require the review and approval of the Grants Officer.

iii. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and II.E.1.c of this BAA.

e. Conference and Symposia Grants

i. Introduction. The Army supports conferences and symposia (as defined in the DoD Travel Regulations) in areas of science that bring experts together to discuss recent research or educational findings or to expose other researchers or advanced graduate students to new research and educational techniques. The Army encourages the convening in the United States of major international conferences, symposia, and assemblies of international alliances.

ii. Eligibility. Notwithstanding the Army's authority to provide grant support for such events, only non-commercial scientific, technical, or professional organizations that qualify for tax exemption may receive a conference grant/symposia grant. Those who meet this requirement should also be aware that the DoD does not permit "co-sponsorship" (as defined in DoD 5500.07-R) absent additional high level staffing and approval. In other words, the conference grant support identified in this BAA is NOT DoD sponsorship or co-sponsorship since ARL/ARO is neither an organizer, nor provider, of any substantial logistical support for the conferences addressed in this section.

iii. Conference Support. Conference support proposals should be submitted a minimum of six (6) months prior to the date of the conference.

iv. Technical Proposal Preparation. The technical portion of a proposal for support of a conference or symposium should include:

(1) A one page or less summary indicating the objectives of the project.
(2) The topics to be covered.
(3) The location and probable date(s) and why the conference is considered appropriate at the time specified.
(4) An explanation of how the conference will relate to the research interests of the Army and how it will contribute to the enhancement and improvement of scientific, engineering, and/or educational in general and activities as outlined earlier in the research areas of this BAA.
(5) The name of chairperson(s)/(PI)(s) and his/her biographical information.
(6) A list of proposed participants and the methods of announcement or invitation.
(7) The number of Army personnel who will be admitted to the conference without charge. Optional- This information is for Army planning purposes, and will not affect evaluation of the proposal.
(8) A signed cover page.

v. Cost Proposal Preparation. The cost portion of the proposal should show:

(1) Total project conference costs by major cost elements.
(2) Anticipated sources of conference income and amount from each.
(3) Anticipated use of funds requested.
(4) A signed budget.

vi. Participant Support. Funds provided cannot be used for payment to any federal government employee for support, subsistence, or services in connection with the proposed conference or symposium.

vii. Cognizant ARO TPOC/ Program Manager. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of a conference/symposia proposal.

f. High School Apprenticeship Program (HSAP)/Undergraduate Research Apprenticeship Program (URAP)

i. The HSAP funds the Science, Technology, Engineering, and Mathematics (STEM) apprenticeship of promising rising high school juniors and seniors to work in a university structured research environment under the direction of ARO sponsored PIs serving as mentors. The URAP provides similar opportunities for undergraduate students. HSAP and URAP participants must be U.S. citizens or have permanent resident status. Awards will be made as add-ons to research grants, Multidisciplinary University Research Initiative (MURIs), University-Affiliated Research Contracts (UARCs), and cooperative agreements that have at least 12 months period of performance remaining from the date of HSAP/URAP proposal submission.

ii. HSAP/URAP program goals are to:

(1) Provide authentic science and engineering research experience to high school students interested in pursuing STEM, and undergraduate students pursuing science and engineering majors;
(2) Introduce students to the Army's interest and investment in science and engineering research and the associated educational opportunities available to students through the Army's Educational Outreach Program (AEOP) and DoD;
(3) Provide students with experience in developing and presenting scientific research;
(4) Provide students with experience to develop an independent research program in preparation for research fellowships, graduate school, and careers in science and engineering research;
(5) Provide opportunities for the student to benefit from the expertise of a scientist or engineer as a mentor for professional and academic development purposes; and
(6) Develop student's skills and background to prepare them for competitive entry to science and engineering undergraduate programs

iii. The HSAP/URAP is designed as an add-on to larger research projects and limited funding is available annually for PIs interested in participating. Due to the brief duration of the HSAP/URAP and limited funding we make every effort to maximize the number of student apprenticeship opportunities. PIs should submit a short proposal that clearly articulates the meaningful research that the student will conduct, along with the strategy for mentorship and facilitation of follow-on opportunities (e.g., university attendance, participation in other AEOP opportunities and other research experiences, etc). PIs must determine what aspect(s) of their current research program the student will be working on, desired deliverables, and anticipated research outcomes (based on the HSAP/URAP program goals in f. ii. of this section). PIs should describe who within their organization will be responsible for day-to-day mentoring of the students (e.g. PI, research associate, graduate student, etc.). If direct supervision of students will be someone other than the PI, the mentor's resume or curriculum vitae (CV) must be provided. The proposal should identify the gains for the student and the organization for HSAP and URAP participation in terms of technical skills, scientific reasoning in specific domains, or publication opportunities. Follow-on opportunities and relationships for students within the organization are encouraged.

Proposals should include provisions to pay HSAP students a stipend equivalent to approximately $10 per hour and URAP students a stipend equivalent to approximately $15 per hour; not to exceed 300 hours total per student. Students are not considered university employees whose hours must be tracked and therefore stipends are not required to be paid as an hourly wage but can be paid as a lump sum or divided as partial payments, at the university's discretion. Proposals should generally be limited to two students per PI, except for UARC and MURI awards on which up to 6 students are allowed. Up to four students will be considered under a single investigator if the proposal demonstrates sufficient senior research staffing to ensure effective student guidance and mentoring. Student stipends must be listed under "participant support costs" on ARO Form 99 as described in Section II.H.2.e of this BAA.

If more than one student is proposed by a PI, there must be a near equal mix of HSAP and URAP (i.e. proposals should not be for multiple URAP students only unless approved by ARO). The institution of higher education must describe in its proposal how it will ensure the protection of minors through provision of a safe working environment.

(1) Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.e and II.E.2.c-d of this BAA.

(2) Describing an Outreach Strategy and Student Application Process. A primary objective of the HSAP and URAP is to expose new students to research opportunities in a research laboratory. Thus, PIs must describe a plan to attract and engage students not related to the PI (family member) or already working with the PI, laboratory, or research project. The proposal shall also include a short description (3 to 5 sentences) of the project and specific student requirements (GPA, letters of recommendation, dates of the apprenticeship, etc.). For approved proposals, the project description and requirements submitted by the PI will be marketed on the AEOP website and used in addition to the PIs outreach strategy to attract applicants. All student applications for the HSAP and URAP programs must be collected through the AEOP student application portal (www.usaeop.com). After initial AEOP eligibility screening, applications will be forward to the PI for evaluation and final candidate(s) selection. PIs must include in the proposal a plan to conduct local outreach to promote awareness of the opportunity among students/schools, and then direct them to the AEOP website to apply. HSAP/URAP is a commuter program and PIs are encouraged to perform outreach to students who are able to commute daily. PIs and mentors must also complete a brief registration annually on the AEOP website and complete a 21st Century

Skills Assessment for each apprentice during the apprenticeship (web links will be emailed to the PI before the start of the summer program). At the conclusion of the apprenticeship student participants are required to develop a brief (one-page) abstract of their work to be included in an AEOP program booklet. PIs shall review and approve these abstracts before submission to ARO.

(3) Timeline. Consistent with the BAA, proposals are accepted on a rolling basis. PIs interested in receiving HSAP/URAP funding should submit proposals no later than (NLT) September 30 of the prior year to provide sufficient time for proposal review, award processing, and student outreach/recruitment. For example, to receive funding for use in summer 2020, proposals should be submitted by September 30, 2019. PIs will be notified of proposal evaluation results by mid November and student application website will open during the first week of January through the end of February.

(4) Proposal Submission. Proposals should not exceed three pages (excluding supplemental information (budget, CVs, etc.) in length and must be submitted through www.grants.gov utilizing solicitation number W911NF-17-S-0002. Complete forms Standard Form (SF) 424, ARO Form 99 (clearly distinguishing high school students from undergraduates), and upload the proposal as an attachment. Please include the title of the research project, the grant number, and the specific number of HSAP and/or URAP opportunities requested on the first page of the proposal.

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g. Historically Black Colleges and Universities and Minority-Serving Institutions (HBCUs/MIs)

The Army has a long history of advocating and supporting research at HBCU/MIs. Through this BAA, the CCDC's Army Research Office actively seeks proposals from the HBCU/MI community in full and open competition with all applicants. Proposals may relate to any research topic described herein. In addition to single investigator research proposals, collaborative research proposals are also encouraged. Collaborations may be between HBCU/MIs and other institutions of higher education (not limited to HBCU/MIs) and/or partners. Also included are special emphasis programs such as STIR and the YIP, described in detail elsewhere in this announcement.

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